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A. Chemistry

Composite Alginate Gels with Embedded Polylactide Nanoparticles as New Controlled Release Systems

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The research and application of new forms of nanotechnology products represents a very promising area, which can seriously advance the medical practice. The injectable hydrogel based systems enabling to perform zero-order controlled drug release are of special interest. Such systems could be indispensable for the long-time treatment of hard-to-reach parts of the organism, for example, at post-surgical brain cancer chemotherapy.

The alginate hydrogels are interesting and well-studied polymer systems that can be used for controlled release of various drugs via diffusion-controlled mechanism. Nevertheless, the drug release from flexible hydrogel is quite fast and reaches nearly 100% within a few hours. For some applications, the time of release has to be substantially prolonged.

In the present study the new type of biodegradable composite hydrogels was designed to raise efficiency and duration of encapsulated drug release. Alginate hydrogels were prepared with two kinds of loading material: model drug molecules itself and PLA nanoparticles containing drug. These PLA nanoparticles were prepared by nanoprecipitation and double-emulsion methods. Proper conditions, such as polymer and drug quantities, kind of binder and its concentration, nanoparticles load etc., were investigated to prepare and sew hydrogels containing different kinds of load. Synthetized hydrogels were described by their swell ratio, drug loading etc.

In order to evaluate the possibility of application of obtained hydrogels as drug delivery systems, a series of experiments were performed to evaluate the kinetics of model drug (Cardiogreen®) release. The quantity of released Cardiogreen® was estimated spectrophotometrically and its release profiles from just alginate hydrogel and composite one were determined and compared.

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Development of the Technique of Arc Emission Spectral Analysis of Fish Tissue with Pre-Mineralization

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Fish is a very important part of a healthy diet, it is a good source of high quality protein and contains very little saturated fats and fatty acids, thereby making its consumption essential for a healthy diet. However all toxic substances, which fish contains, transfer into the human body and might damage the organism. Consequently, heavy metals accumulated in marine objects are transmitted to humans through food chains. Due to top position of fish in food chains of aquatic ecosystems, it is a fine biological indicator of environmental pollution with a number of substances.

Marine pollution with heavy metals became a very urgent problem in modern world not only for the threat of extinction of various fish species, but as well as possible health risks for fish-consumers. A great attention is given to a number of toxic elements such as Hg, Pb, Cd, As. For instance, Pb causes kidney failure and cirrhosis, furthermore long-lasting Pb intake can lead to coma condition, mental deficiency and even death. Other metals (for example Cr, Zn, Cu) cause nephritis and severe kidney damage. Consequently the problem of environmental pollution with heavy metals in aquatic ecosystems cannot be omitted. Also it is important to determinate levels of Ca, Mg, P, which are essential to human body. Therefore it is advantageous to use the methods of multielement analysis, for example digital atomic emission spectrographic analysis with the excitation spectrum of solid residue samples from the end of the carbon electrode in the a.c. arc.

The majority of techniques of the analysis of such objects offered by researchers include pre-mineralization for the purpose of obtaining liquid samples. Despite the fact that there are lots of articles describing methods of mineralization applicable to our subject, they vary in execution time and chemical reagents. This study included experimental comparison of methods of wet mineralization, selection of the optimal one and its further improvement for subsequent determination of heavy metals, essential and other elements in the resulting mineralizators. Results of optimization made to the technique of emission spectral analysis with a purpose of improvement the analytical characteristics are also presented. The accuracy was confirmed by a standard reference material. Developed methodology was used for identification of the elemental composition of fish tissues and evaluation of the detected elements.

Part of the research was done using the equipment of the Educational Resource Center of Chemistry of Research Park of St. Petersburg State University.

Gaseous Lead Phosphates: Structures and Thermodynamic Properties

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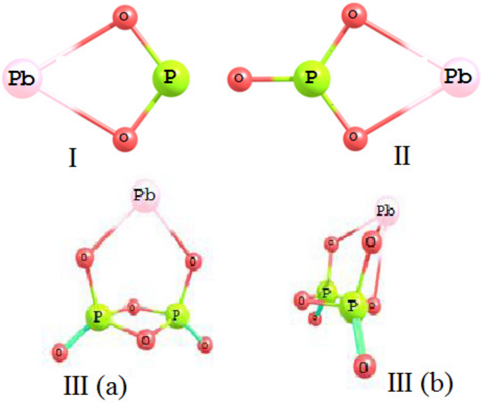
Phosphates of elements of 14 group are perspective materials for construction of new types of fireproof materials, stable covers, antirust coatings and glasses for specific purposes [1].

Our research team has investigated vaporization processes of $Pb(PO_3)_2$ and $Pb_2P_2O_7$ in neutral and reducing conditions in temperature range of 1400-1600 K. To determine the partial pressures of vapor species over the samples high-temperature Knudsen effusion mass spectrometry method was used. Measurements were performed with a MS-1301 mass spectrometer. A theoretical study of gaseous lead phosphates was carried out by several quantum chemical methods: wave function based explicitly correlated F12 methods and DFT M06 methods. Energetically favorable structures were found (Fig. 1) and vibrational frequencies were evaluated in the harmonic approximation.

The formation enthalpies of gaseous $PbPO_2$, $PbPO_3$ and PbP_2O_6 were obtained. For this purpose we have determined the enthalpies of a numerous gas-phase reactions involving gaseous lead phosphates. Experimental data are in an agreement with those evaluated theoretically.



I

II

III (a)

III (b)

Fig. 1. Structures of gaseous I - $PbPO_2$, II - $PbPO_3$, III (a, b) - PbP_2O_6.

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Effervescence Assisted Dispersive Liquid-Liquid Microextraction Followed by Microvolume UV-vis Spectrophotometric Determination of Surfactants in Water

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Green analytical chemistry provides the development of the various analytical procedures and methods with a minimal impact on operators and the environment. Green sample pretreatment approaches, especially microextraction, have been found the great attention as they lead inherently to a minimum solvent and reagent consumption and drastic reduction of laboratory wastes.

Nowadays, despite the environmental toxicity, surfactants are widely used in both domestic and industrial areas. For the determination of surfactant spectrophotometry is usually used. This procedure is based on the ion-pair extraction of surfactant with organic dye into a suitable organic solvent. Unfortunately, the volumes of the solvent required for the extraction are very large which contradicts the concept of Green chemistry. This problem is possible to solve by the using of dispersive microextraction.

The novel and simple methods for the sensitive determination of cationic and anionic surfactants in water based on effervescence assisted dispersive liquid-liquid microextraction (EaDLLME) and microvolume UV-vis spectrophotometry have been developed. The method is based on the ion-pair extraction of cationic and anionic surfactants with organic dyes – methyl orange and azure A, respectively, into $CHCl_3$ using EaDLLME technique. The EaDLLME assumes the dispersion of $CHCl_3$ by CO_2 bubbles, which are formed by the injection of acetic asid and $CHCl_3$ mixture into sample solution which contain carbonate-ions.

EaDLLME procedures have LOD values 0.03 mgL^{-1} and linear range for concentrations 0.1–5.0 $mgL^{-1}$for both cationic and anionic surfactants. Moreover, the EaDLLME is ecological friendly, because it does not require using of additional organic solvent. The main advantage of EADLLME is its rapidity and less time consuming because there is no need to use centrifugation step for cloudy state agglomeration.

Phosphine-Alkynyl Heterometallic Hybrid Systems Au-M (M = Cu, Ag) as the Precursors for Synthesis of Self-Organizing Surfaces and Nanoparticles Au-Ag@C

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Recently, the nanocomposite materials, which contains the nanoparticles of precious metals, dispersed in a carbon matrix, attract the increasing attention of many researchers. At the same time, self-organized monolayers on surfaces attract the growing interest due to bright photophysical properties. Herein we report precursors for both motivations that can be easily prepared according to the following scheme (Fig. 1):

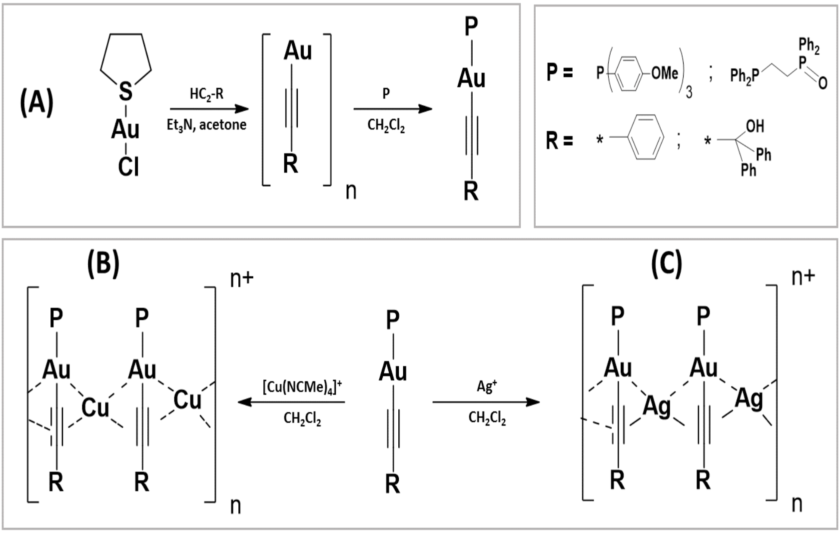

Fig. 1. Synthesis of the precursors.

The structures of (A) in solid state and solution were established by NMR spectroscopy and XRD analysis. Photophysical properties of (A), (B) and (C) were investigated. Excitation and emission spectra of (B) and (C) clearly demonstrate some radical changes with introduction of heterometal in (A). Self-organizing materials on aerosil surfaces based on (B) and (C) were received. Lazer deposition of (C) in solution led to formation of Au-Ag@C nanoparticles.

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Chemical Equilibrium and Thermal Effects of Ethyl Acetate Synthesis Reaction at Polythermal Conditions

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The study of the phase and chemical processes in systems with reactions and stratification is important for the applied aspects of science and development of fundamental thermodynamic theory. For example these processes are rather wide applied in chemical technology and for development of industrial organic synthesis. The thermodynamic study of such a systems is of particular interest. A lot of previous studies of phase equilibrium provide data on the liquid-liquid and liquid-vapor equilibriums, but only a limited number of them consider the systems with a chemical reaction. The set of investigations of the liquid-liquid phase equilibrium with simultaneous chemical reaction is presented in the papers [1-2]. These works report data on the solubility (20, 30 and 40°C), the liquid-liquid phase equilibrium (20, 30 and 40°C), as well as the chemical equilibrium (20, 30ºC) for a system acetic acid - ethanol - ethyl acetate – water. Here we report the results of study of chemical equilibrium in this system at several temperatures (40 and 50°C) and the data on the thermal effects of the esterification reaction and the heat of mixing of the two starting components (obtained by calorimetric methods of analysis). The experimental data on chemical equilibrium was obtained by two different methods: gas chromatography and nuclear magnetic resonance spectroscopy.

Acknowledgements

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Synthesis of Arylboronic Acids Using Acyclic Diaminocarbene Complexes of Pd(II) as Catalysts

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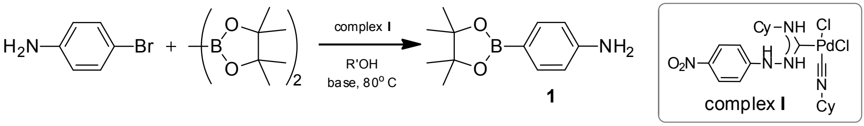
Arylboronic acids are reagents for Suzuki reaction, which is the most important cross-coupling synthetic methodology to prepare diverse biaryls and heterobiaryls. The typical preparation of arylboronic acids or esters involves the reaction including aryllithium compounds or Grignard reagents. However, the method is difficult to apply for substrates bearing some heterocycles or functional groups that are not compatible with organolithium reagents.

In 1995, Miyaura pioneered the Pd-catalyzed borylation of aryl halides without the use of organometallic reagents [1]. Large amount of experimental data has been since obtained, though the most successful methods still include using biohazard solvents, such as DMSO, THF, dioxane etc, inert atmosphere and catalysts, that are difficult to obtain [2-5].



In this work we managed to optimize the reaction conditions as following: alcohol solvents, which are relatively harmless, available and mild bases (KOAc, K_2CO_3), no inert atmosphere, low quantity of catalysts (0.1 mol% compared to 3-5% in literature).

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Engineering Nanoporous Iron(III) Oxide into an Effective Water Oxidation Electrode

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The ability to electrolyze water into its elements in benign conditions at low cost will imply the exclusive use of cheap, abundantly available materials, instead of most advanced catalysts.

Here, we demonstrate that iron oxide, the most abundant and least expensive transition metal compound, can be used as a catalytically active surface for the four-electron water oxidation to O_2 at neutral pH which represents the kinetic bottleneck of the overall reaction. The geometric effects of nanostructuring a pure Fe_2O_3 surface on its electrochemical water oxidation performance were systematically explored. Atomic layer deposition was used to coat the inner walls of cylindrical “anodic” nanopores ordered in parallel arrays with a homogeneous Fe_2O_3 layer. Combining electrochemical treatments with the “anodic” pore geometry delivered an effective increase in turnover by a factor of 65 with respect to a smooth, planar Fe_2O_3 surface (Fig. 1). However, the current density depended on the pore length in a non-monotonic manner. An optimal length was found that maximized turnover by equating the rate of transport in the electrolyte with that of charge transfer across the interface.

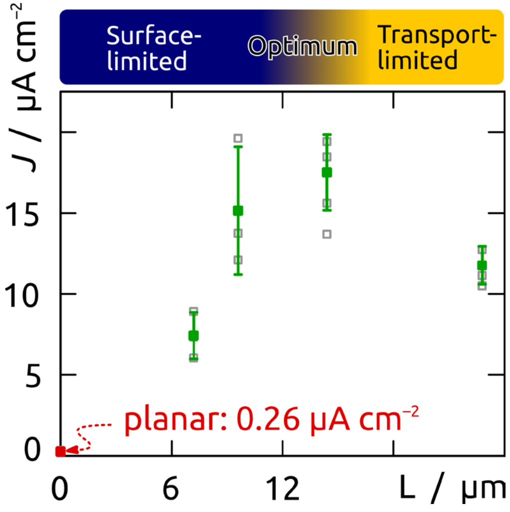

Fig. 1. Geometric optimization of nanoporous Fe_2O_3 electrodes for water oxidation at pH 7.

SERS Study of Adsorption of New Acridine-Based Fluoroinophore on Silver Colloid

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Surface-enhanced Raman spectroscopy (SERS) is a powerful tool for surface chemistry and physics investigation. In terms of adsorption chemistry SERS is particularly valuable because there are no alternative locally sensitive methods for the investigation of adsorbate state. The study of adsorbates by SERS spectroscopy provides information about their transformations on the surface and interaction with the solution components [1].

In this work we present the investigation of adsorption of newly synthesized acridine derivative 4,5-bis(N,N-di(2-hydroxyethyl)iminomethyl)acridine (BHIA) on silver colloid. BHIA is high selective fluorophore to Cd^{2+} cations [2], the study of its interaction with SERS-active surface is interesting not only from a practical point of view in order to develop an optical sensor, but also in terms of proposing the model of adsorption. For BHIA due to the bulky substituents a direct interaction of the molecule via nitrogen atom of acridine fragment with the surface is limited on the one hand, the aliphatic substituents themselves may interact with the silver surface through hydroxyl groups on the other hand. Halide anions are known to capable of activating a silver surface that leads to great enhancement of SERS intensity [3]. In the SERS spectrum of BHIA adsorbed on silver colloid not only the enhancement of intensity occurs but also an alteration of its profile after KCl addition to the solution. The observed in SERS spectra changes we attribute to the transformation of physisorbed BHIA species to chemosorbed.

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Laser-Induced Method of Synthesis of Hybrid Metal-Carbon Nanostructures on the Surface of Dielectrics and Semiconductors

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At the modern technological time, there is a strong demand to developed novel functional materials consist in combination of different matters in a single species to give so-called hybrid materials. Natural hybrid materials often possess complex, hierarchical architectures at sizes ranging from a few nanometers to several micro- or millimeters. Their collective properties are determined by the combination of both the structure and composition on each length scale.

In this work we present an approach to the synthesis of hybrid metal-carbon nanostructures on the different surface. The method is based on laser-induced heterogeneous photochemical reaction. The process of hybrid nanostructures preparation by laser irradiation of interface liquid phase/solid phase is single-step. The hybrid nanostructures formation occurs throw the generation and growth of nucleus during the irradiation of the substrate in chemically active liquid. Focused laser beam allows to act locally on the interface and focal volume designates the region of laser-induced chemical reaction. Scanning of the interface by laser beam gives the possibility to create the hybrid nanostructures with difficult architecture.

We have demonstrated a simple, flexible and highly versatile approach to fabricate hybrid metal-carbon nanostructures on the surface of dielectrics and semiconductors.

The reported study was supported by Ministry of education and science of Russia within project 14.604.21.0078 (registration number RFMEFI60414X0078). All measurements were carried out at Center for Optical and Laser Materials Research and at the Interdisciplinary Resource Center for Nanotechnology.

Design of Water Soluble Luminescent Rhenium(I) Complexes

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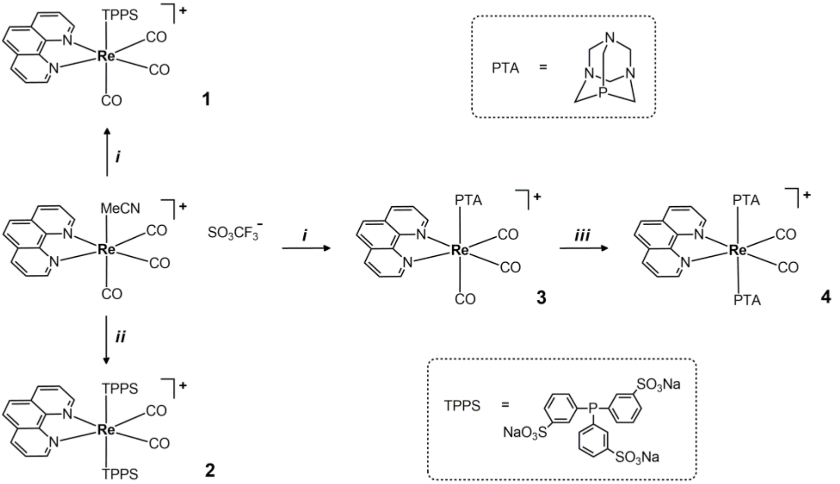
The luminescent organometallic compounds have been attracting great attention during the last two decades. The recent exponential growth of this area has been particularly stimulated by the strong expectations that the properties of luminescent metal complexes will make breakthroughs towards a number of modern and important technological applications.

Here in we report an overview of four novel water soluble rhenium(I) complexes. They have been prepared according to the following scheme:



Reaction conditions: ***i*** *– 110-130 °C, autoclave;* ***ii*** *– 220 °C, autoclave;* ***iii*** *– photolisys and reflux in acetone.*

All complexes were characterized by ^{1}H and ^{31}P NMR spectroscopy, IR spectroscopy, and by mass-spectrometry (in a solution), and by X-ray diffraction analysis (in solid state).

Due to different nature of phosphorous ligands the biological transport properties of complexes 1−4 can differ as well. Interestingly obtained complexes are performing better as light emitters (longer lifetimes and higher quantum yields) in water than in methanol which is a good starting point for their applications *in vivo.*

New Complexes of Pd(II) and Pt(II) with 1-phenil-1,4-dihydrophosphinolines Ligands

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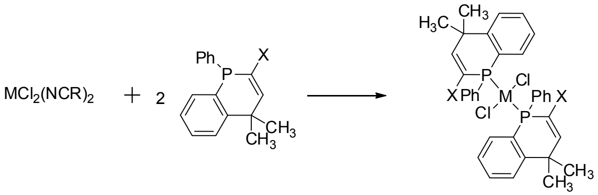
Complexes of platinum and related metals such as Pd, Ir, Rh, Ru contained phosphine ligands are widely employed in homogeneous catalysis as well as getting used to being attractive candidates for a theoretical study [1]. A few examples *viz.* 1,4-dihydrophosphinolines **1a,b** of a new class of heterocyclic phosphines have been obtained and fully characterized in our laboratory recently. Here we report on the synthesis of Pd(II) and Pt(II) complexes contained phosphine ligands mentioned above and full account study of their structure in solid state as well as in the solution.

Reaction between nitrile complexes $[PdCl_2(NCCH_3)_2]$ (**2**) and $[PtCl_2(NCCH_2CH_3)_2]$ (**3**) with phosphines **1a,b** proceeds in CH_2Cl_2 at r.t. for *ca.* 1 d giving the $[MCl_2P_2]$ species **4–7** in good (82–94 %) isolated yields (Scheme 1).



M = Pd, R = CH_3 **2**
M = Pt, R = C_2H_5 **3**

X = H **1a,**
X = Br **1b**

M = Pd, X = H **4** 82 %;
M = Pt, X = H **5** 87 %
M = Pd, X = Br **6** 86%;
M = Pt, X = Br **7** 94 %

Scheme 1. Synthesis of complex **4–7**.

Complexes **4–7** were characterized by high resolution ESI$^+$-MS, ^{1}H, ^{13}C{^{1}H, ^{31}P}, ^{31}P and ^{195}Pt NMR spectroscopies. In addition, the structures of all complexes were elucidated by a single-crystal X-ray diffraction.

This work has been partially supported by Russian Foundation for Basic Research (grant 14-03-31204 mol_a). Physicochemical studies were performed at the Center for Magnetic Resonance, Center for X-ray Diffraction Studies, and Center for Chemical Analysis and Materials Research of Saint Petersburg State University.

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Development of the Technique of Arc Emission Spectral Analysis of Cigarette Tobacco with Pre-Mineralization

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Tobacco smoking has been ranked among the world's preventable cause of death, because from 3.5 to 5.4 million people die annually as a result of health problems caused by smoking. Most of the people know what damage to health nicotine and tar (basis of tobacco) cause. But besides them tobacco contains heavy metals, which could provoke irreparable harm. As far as tobacco smoke is directly contacts with the lungs, these elements easily penetrate into the human organism.

Many heavy metals, such as Fe, Cu, Zn, Mo involve in biological processes and in certain amounts are necessary for the normal functioning of plants, animals and humans. On the other hand, some heavy metals and their compounds are carcinogenic. A lot of metals, including essential, can accumulate in tissues and organs, causing some diseases and disastrous impact on the human organism. For example, an excessive content of Pb (the presence of which has been proved in tobacco) in the body leads to the affection of the hematopoietic and nervous systems, kidneys. High content found in tobacco Cd results in increasing of the risk of "earn" lung cancer, a renal dysfunction, an increase blood pressure, and then a stroke. Therefore the determination of heavy metals in tobacco is an important problem of modern toxicology.

Mostly all modern highly sensitive and most commonly used analytical methods require complex sample preparation, including mineralization of samples. In the literature there are a large number of substantially different (in duration, equipment and reactants used) performances of this step. The purposes of this study are the experimental comparison of different ways of sample mineralization, choosing the most preferred one and its optimization for subsequent determination of heavy metals and other elements in mineralized samples. Developed technique was verified by analysis of standard reference material of grass. Identification of the tobacco elemental composition and assessment of the content of detected elements are also presented. Data in this study was obtained by means of alternative to ICP-AES and ET-AAS method – a.c. arc AES analysis of liquid samples, previously developed in our laboratory.

Part of the research was done using the equipment of the Educational Resource Center of Chemistry of Research Park of St. Petersburg State University.

Molecular Complexes of Lewis Acids with Polydentate Donors

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Strong Lewis acids such as group 13 element trihalides form stable molecular donor-acceptor (DA) complexes with polydentate donors, such as pyrazine. In the present work, complexes $(GaI_3)_2$pyz and GaI_3pyz have been synthesized and structurally characterized (Fig. 1). In contrast to polymeric $(GaCl_3pyz)_\infty$, complex GaI_3pyz is a monomer with tetrahedral geometry of gallium atom [1]. Acording to the Cambridge Crystallographic Data Centre database, structural data for only three other pairs of molecular DA complexes of 2:1 and 1:1 composition are available. This allows direct comparison of the structure and energetics of the first and second DA bond. Computational studies of these pairs of complexes have been carried out at B3LYP/def2-SVP level of theory and indicate that the second DA bond is weaker than the first, which is in good agreenment with trends in DA bond distances found experimentally.

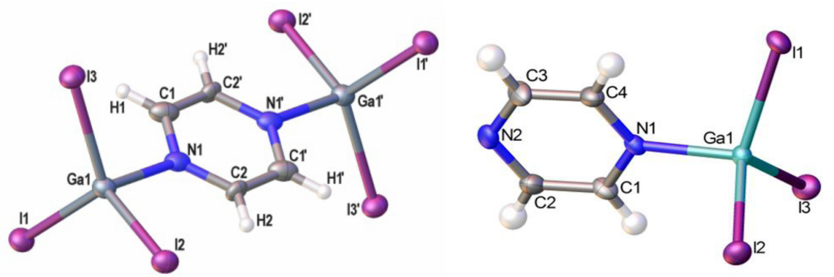

Fig. 1. Molecular structures of complexes $(GaI_3)_2$ pyz (left) and GaI_3pyz (right).

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Interaction between α-Aminoazoheterocycles and Palladium(II) Coordinated Isocyanides

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Metal complexes with aminocarbenes are widely employed in catalysis of various organic transformations as a powerful alternative to the commonly used phosphine complexes. Generation of aminocarbene complexes can be achieved via several distinct routes and the most promising approach involves metal-mediated addition of N-nucleophiles to metal-bound isocyanides. In our research group it was previously found that addition of palladium(II) isocyanides complexes to α-aminoazaheterocyles leads to aminocarbene complexes which themselves are nucleophiles and able to attack another isocyanide complex with the formation of binuclear complexes.

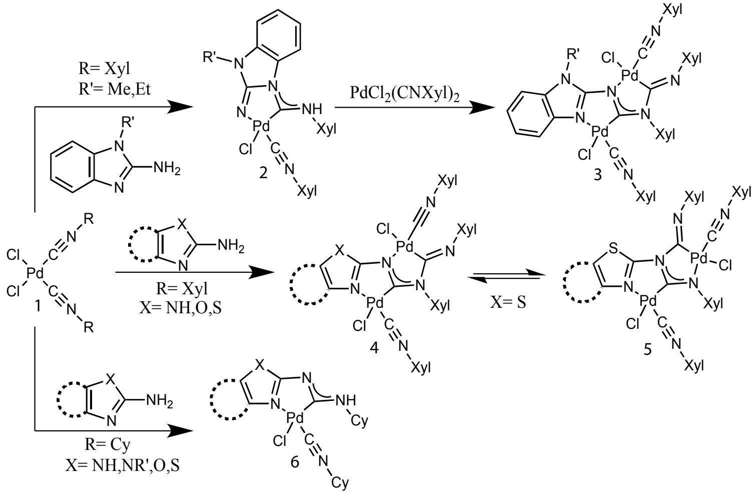

Fig. 1. Interaction between α-aminoazoles and Pd(II) isocyanide complexes.

In this research we have studied the relationship between the structure of carbene complex and nature of isocyanide ligand and α-aminoazaheterocyle.

Acknowledgements

Physicochemical studies were performed at Magnetic Resonance Research Center, Center for X-ray Diffraction Studies and Chemical Analysis and Materials Research Center of SPbU. The authors thank Russian Foundation for Basic Research (grant 14-03-31204 мол_а, 14-03-00297а) and SPbSU (grants 12.38.225.2014, 12.38.195.2014).

Adsorption of Bovine Serum Albumin onto Modified Polylactide Films

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The formation of macroporous 3D structures (named *scaffolds*) is based on biocompatible polymers and is intended to be used in autologous tissue regeneration which is a reasonably important part of modern biomedical materials research area [1]. Such scaffolds should contain special biofunctional motifs on their surface in order to promote cell adhesion and differentiation. In this study we propose the application of polymers with «molecular sites» – specific binding sites, formed via molecular imprinting (MI) strategy and capable for reversible binding of cell receptors as a tool for modification of polylactide based scaffolds [2]. The use of the macroporous cryogels as MI system has already shown exceptionally promising results [3].

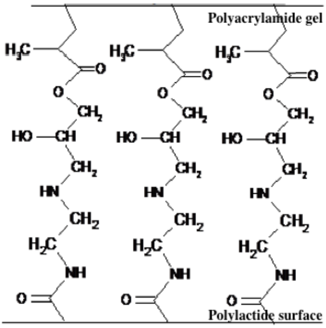

Fig. 1. Structure of modified PLA film.

Thus our aim was to form hydrogel layer on the surface of polylactide and imprint model protein into such layer. For that the films of polylactide (PLA) were made and modified by polyacrylamide gel (PAAg) (Fig. 1) with and without template - bovine serum albumin (BSA) molecule and then put in the BSA solutions for adsorption study. Films surfaces were analyzed by SEM method and contact angle measurements, adsorption and desorption processes were studied (Fig. 2). The experiments has shown that BSA tends to form multilayers on PLA surface which gradually saturates and gladly desorbs, unlike PAAg which never does any of those (BSA concentration 1 – 30 mmol/l) as it has lots of pores and they hold a sufficient amount of protein.

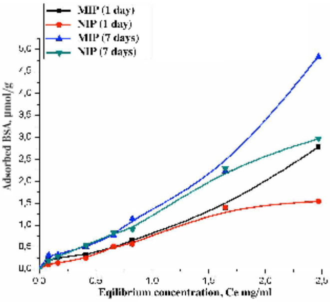

Fig.2. Adsorption isotherms.

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Al and Sc Doped TiO_2: Photocatalytic Activity

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Metal doping is a promising way to enhance the activity of photocatalysts. The optimal metal dopant concentration for a catalyst of a given particle size was shown [1] to vary from 0.01% to 1% independently on the metal dopant nature.

In the present work a series of Al and Sc doped titanium dioxide samples synthesized by sol-gel and solid state methods was studied. Surface characterization was carried out by SEM, X-ray phase analysis, BET and FTIR spectroscopy of adsorbed CO. Photoactivity was evaluated by phenol decomposition under irradiation in aqueous suspension.

The dependence of initial phenol decomposition rate on the weight percentage of aluminum manifests a maximum at 0,5% of Al content and shows the activity higher than for commercial P25 TiO_2.

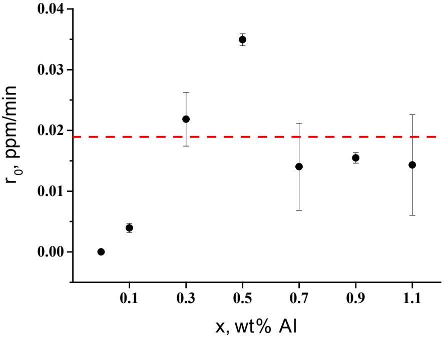

Fig. 1. Phenol degradation rate (r_0) on the aluminum percentage (x). Dashed line - degradation rate for commercial TiO_2 Evonik P25.

Regarding scandium the optimal concentration seems to be above 1,1 %, since we observed the increase of activity from 0,1 % to 1.1 % samples.

Aluminum and scandium doping seems to be a promising way to improve the quality of titania based photocatalysts. This study may also contribute into understanding the mechanism of metal doped materials photoactivity.

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Reduction of Oxygen at a Poly[Pd(Salen)] Modified Electrode in Alkaline Media

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Nowadays, the demand for an efficient fuel cell is bigger and bigger. On the cathode in fuel cells occurs the oxygen reduction reaction (ORR) and ORR would be kinetically slow without any catalyst. Platinum-based materials are known for its good catalytic activity in ORR and for its expensiveness. Therefore, it's very important to invent good catalysts in ORR.

The catalytic activity in ORR of glassy carbon electrodes modified by a polymer film of palladium complex with a Schiff ligand, PdSalen (Fig. 1.) was studied in an alkaline aqueous solution with cyclic voltammetry. Although its catalytic activity was worse than even the one of glassy carbon itself, it showed a better activity than glassy carbon after being applied higher potential for some minutes.

The Koutecky-Levich plot of the oxidised PdSalen polymer suggested that the number of electrons in ORR decreased with decreasing the potential. It means the reduction pathway changed. It might be caused with a transformation of the complex.

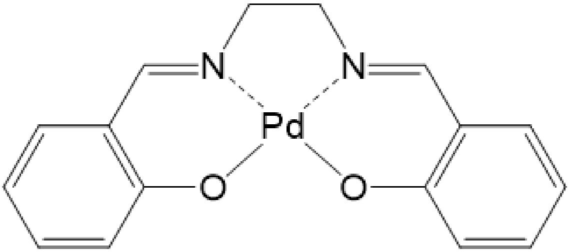

Fig. 1. PdSalen.

The Influence of Exciplex Formation on the Photophysics of a Series of Dinuclear Au(I)–NHC Complexes

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The stimuli-responsive nature of auro- and metallophilic interactions is currently emerging as a versatile tool in the development of various sensing applications including ion probes, environmental sensors and biomedical diagnostics. Being weak dispersion forces, metallophilic interactions are perfectly suited to form the basic machinery through which relevant analytical signals can be transduced with the added benefit of relatively simple optical detection.

Our current research efforts are directed at understanding the basic mechanisms of the unique stimuli-responsive behavior characteristic of aurophilicity-augmented species, and, in this vein, we carried out an in-depth experimental and theoretical investigation of a series of dinuclear Au(I) bis(carbene) complexes (Fig. 1).

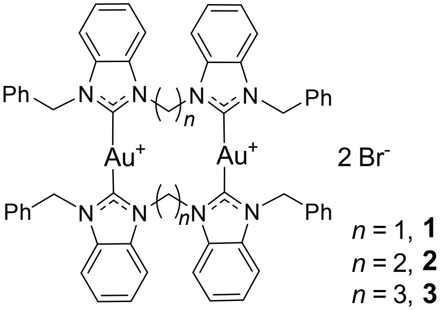

Fig. 1. The general structure of the investigated complexes.

It was found that, in solution, the emission profiles of the compounds under study were markedly different from each other and dependent on the presence of excess bromide. The addition of excess bromide to the solutions of complexes **1** and **3** leads to red shifts of *ca* 60 nm, while in case of the ethylene-bridged complex **2**, which is non-emissive when neat, green luminescence emerges. A detailed computational study undertaken to rationalize the observed behavior revealed the determining role aurophilicity plays in the photophysics of these compounds, while the formation of exciplexes between the complex cations and solvent molecules or counterions was demonstrated to significantly decrease the Au–Au distance in the triplet excited state. A direct dependence of the emission wavelength on the strength of the intracationic aurophilic contact allows for a controlled manipulation of the emission energy by judicial choice of counterion and the linker length of a diNHC ligand.

A Fully Automated Effervescence-Assisted Switchable Solvent-Based Liquid Phase Microextraction Procedure: Liquid Chromatographic Determination of Ofloxacin in Human Urine Samples

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Fluoroquinolone antibacterial agent ofloxacin (OFLX) is an extensively used drug in the therapy of bacterial infections in humans as well as veterinary medicine. Nevertheless, it can cause a great toxic effect to human body. Because of this point of view, the determination of OFLX in different biological fluids is the highly important task.

Taking into account low levels of OFLX preconcentration of target analyte is a necessary step of sample preparation. Liquid-phase microextraction is one of the most preferable techniques for this purpose, which can be considered under the Green analytical chemistry, since it leads to a minimum solvent and reagent consumption and drastic reduction of laboratory wastes.

A novel fully automated effervescence-assisted switchable solvent-based liquid phase microextraction (EA-SS-LPME) procedure has been suggested for the determination of ofloxacin in human urine samples using high-performance liquid chromatography with fluorescence detection (HPLC-FLD) (Fig. 1). Medium-chain saturated fatty acids were investigated as a switchable hydrophilicity solvents (SHS). The conversion of fatty acid into a hydrophilic form was carried out in the presence of the sodium carbonate. The injection of sulfuric acid into the solution promoted decreasing of pH, thus, microdroplets of the fatty acid were generated. The carbon dioxide bubbles were in-situ generated and promoted the extraction process and finale phase separation.

Under the optimal conditions, the detector response of ofloxacin was linear in the concentration ranges of 0.03-3 μmol L^{-1}. The limit of detection, calculated from a blank test based on 3σ, was 0.01 μmol L^{-1}.

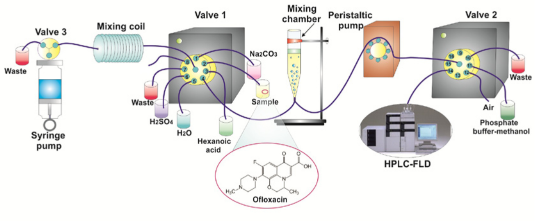

Fig. 1. The manifold for automated EA-SS-LPME system coupled with HPLC-FLD for the determination of ofloxacin in human urine samples.

Mixed Matrix Membranes with Hybrid Star-Shaped Macromolecules for Pervoparation

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Pervaparation is the most promising technology for separation of liquid mixtures due to its highly selectivity, economical, energy-efficient and eco-friendly characteristics. It has been studied extensively because of the potential industrial utility for separation of azeotropic, close boiling, isomeric and heat-sensitive liquid mixtures. Thereby the investigation of novel membrane materials with good transport properties is constantly demanded.

Mixed matrix materials are perspective due to ability to combine benefits of both polymer and inorganic particles. In present work mixed matrix membranes were prepared by involving hybrid star-shaped macromolecules (HSM) (Fig. 1) in polyphenylene oxide matrix and tested in pervaporation of organic mixtures. As a branching center fullerene C_{60} was used.

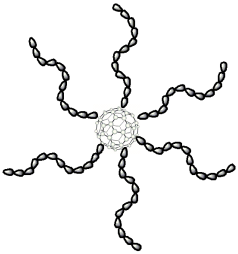

Fig. 1.Hybrid star-shaped macromolecules.

The mixed matrix membranes were characterized by research of morphology and physic-chemical parameters. The results showed that HSM inclusion leads to formation of domains in membranes. The pervaporation experiments were performed using mixtures of methanol and ethylene glycol in different concentrations. The best result was obtained for membrane containing 5 % of HSM.

Acknowledgments

The authors acknowledge the Russian Foundation for Basic Research (project 15-03-02131).

Equipment of the Thermogravimetric and Calorimetric Research Center, Educational resource center of chemistry and Nanotechnology Interdisciplinary Centre of the Saint Petersburg State University was used at the carrying out of the experiments.

Solubility and Chemical Equilibrium in Quaternary Reacting System Propionic Acid - Ethanol - Ethyl Propionate – Water at 20, 30 and 40 °C

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Fundamental research combined reactive mass transfer processes, in which both implemented chemical and phase equilibrium, leading to the establishment of new thermodynamic and kinetic laws [1, 2]. The main task is thermodynamic analysis of the features of liquid-liquid (LL) phase diagrams of the systems with equilibrium and non-equilibrium chemical reaction in solution. The objects investigated are heterogeneous systems with ester synthesis reaction that were carried out both for basic and industrial purposes.

The object of investigation in this research is quaternary reacting system propionic acid - ethanol - ethyl propionate – water. The ternary and binary subsystems (propionic acid - ethyl propionate - water, ethanol - ethyl propionate - water, ethyl propionate - water) were studied.

To study the solubility in stratified system was used isothermal titration method. This method can most accurately determine the position of the binodal. The experimental data on the solubility was obtained at a temperature of 20, 30 and 40 °C. On the base of the experimental data of the solubility in the system investigated the solubility surface was constructed in concentration tetrahedron. Chemical equilibrium was studied at 20, 30 and 40 °C. The experimental data on chemical equilibrium in system investigated was obtained by two different methods: the classical method of gas chromatography and relatively new one for this theme – by nuclear magnetic resonance method. The surface of chemical equilibrium was obtained by gas chromatographic method analysis in the system with ethyl propionate synthesis reaction at 20˚C. The new method of NMR was used to obtain some of the chemically equilibrium compositions at 30 and 40˚C.

Acknowledgements

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Complexes of N-trialkylborazines with Group 13 Metal Halides

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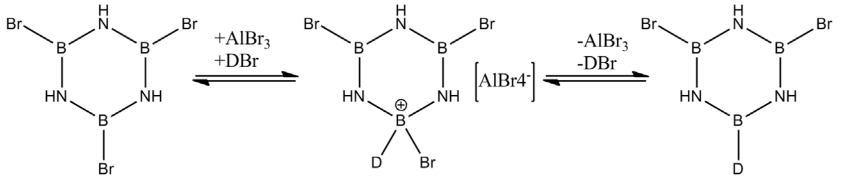
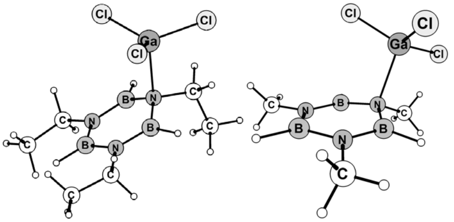
Boron-nitrogen compounds are prospective precursors for ceramic and smart materials [1]. Borazines are isoelectronic to benzene, but in spite of this exhibit quite different reactivity. Recently, the first example of an electrophilic H/D substitution reaction of B,B′,B″-tribromoborazine in deuterobenzene solution was reported in presence of aluminum tribromide [2].



It is interesting if N-substituted borazines can also undergo H/D electrophilic substitution reactions.

In the present report syntheses and characterization of hexamethylborazine and N,N′,N″-trialkylborazines $H_3B_3N_3R_3$ (R=Me,Et) were carried out. Reactions of complex formation with $AlBr_3$ and $GaCl_3$ have been studied both experimentally and theoretically for the first time. Thermodynamic characteristics for complex-formation in solution were obtained by temperature dependent NMR. H/D exchange was not observed. For the gas phase compounds, optimized geometries and complexation energies were established by *ab initio* and DFT computations.



Financial support of SPbSU (project № 12.38.255.2014) is gratefully acknowledged. We thank SPbSU Resource Center for Magnetic Resonance for NMR measurements. Computational resources were provided by Resource Center "Computer Center of SPbSU". We also thank Igor Kazakov for the support and assistance.

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Halogen Bond as Luminescence Amplifier: a Case Study Using Platinum Cyclometalated Complex

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Halogen bonding (XB) is the least explored noncovalent intermolecular interaction. It occurs between an elecrophilic halogen atom in a molecule and nucleophilic region in another or the same molecule. Halogen bonding has a promising potential for application in supramolecular chemistry, material chemistry, organic synthesis and physics [1].

There are very few examples on the effect of XB on the optical properties of transition-metal complexes to date. Herein, we report the first example of the dramatic enhancement of luminescence intensity of a metal complex in the solid state upon formation halogen bonds [2]. The weakly luminescent platinum complex **1** interacts with fluorinated bromo- and iodoarenes forming complexes (Pt-Cl···X-R) in solid state (Fig. 1). The cocrystallization leads to enhancement in the luminescence intensity up to 22-fold.

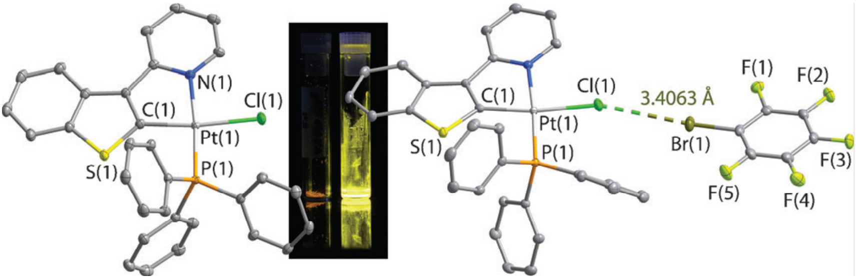

*Fig. 1. X-ray structure of complex **1** (left) and formation of XB between **1** and bromopentafluorobenzene.*

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Mononuclear Au(I) Complexes as Highly Sensitive Sensors for Various Metal Cations

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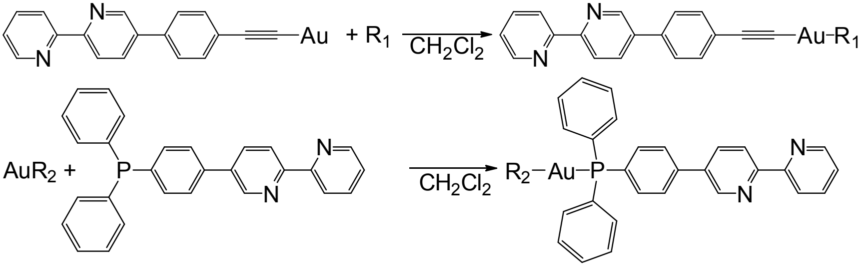
Unique luminescent characteristics of mononuclear Au(I) complexes are currently attracting considerable interest. High sensitivity of luminescence to external stimuli provides opportunity for various sensing applications. Nowadays the quantification of metal cations in different media is becoming more and more important due to the far-reaching implications of metal ions for human health. In cognizance of the immense gravity of the problem we became intrigued by the possibility to utilize gold(I) complexes functionalized with specific cation-binding functionalities as highly sensitive luminescent sensors for various metal cations.

In this study six novel Au(I) complexes based on two new bipyridine-decorated ligands were synthesized. Most of the complexes demonstrate sensitivity to metal cations such as Mg^{2+}, Zn^{2+}, Cd^{2+} and Pb^{2+} and changes in emission are readily perceivable even with naked-eye detection.



$R_1 = PCy_3$, $(C_6H_5)_2P)_2C_6H_{12}$, $CN(o\text{-}(CH_3)_2C_6H_3)$;
$R_2 = C_2C_6H_5$, $C_2C(OH)(C_6H_5)_2$, C_6F_5

The authors greatly appreciate the financial support of St. Petersburg State University research grants 12.42.1458.2015.

Oxygen Reduction Catalysts Based on Platinum Nanoparticles Deposited in Transition Metals Polymer Complexes Matrix

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The reaction of the oxygen electroreduction is the main cathodic process, which occur in the majority of fuel cells. But this reaction has a kinetic limitation, and for it passing the catalyst is needed. The most usable catalysts are the metals of platinum group, but because of expensiveness their usage is limited.

In our work we present a new method of preparation the nanodisperse platinum coatings, modified with nickel (II) complexes with Schiff bases. Obtained materials were investigated by rotating disk voltamperometry, X-ray photoelectron spectroscopy and scanning electron microscopy.

It is shown, that the synthesized catalysts are more effective with respect to electroreduction of oxygen that polycrystalline or nanodisperse platinum.

Scientific research were performed at the: Center for Geo-Environmental Research and Modeling (GEOMODEL) of Research park of SPbSU, Interdisciplinary Center for Nanotechnology of Research park of SPbSU, Center for Chemical Analysis and Materials Research of Research park of SPbSU, Thermogravimetric and Calorimetric Methods of Research park of SPbSU.

Multimetallic Electrocatalytically Active Surfaces

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Creation of electrocatalytically active three-dimensional structures finds its' huge application in different devices such a batteries and fuel cells. For the most effective result it may be used not only three-dimensional structure as a membrane but also the membrane with some nanoparticles inside the pores. The surface area of this object significantly higher than surface of membrane. As a precursor for creating of structures for electrochemistry were used Al_2O_3 membranes with AgAu/C nanoparticles made by laser deposition. The deposition was realized by He-Cd laser with wavelength λ=325nm from thin layer of solution of metalorganic complex. The reaction takes place in the membranes pore as well as on its' surface. For depositing were used membranes with different length and diameter of the pores. These parameters are in dependce of the time of the synthesis. The SE image of such membrane is shown in Fig. 1.

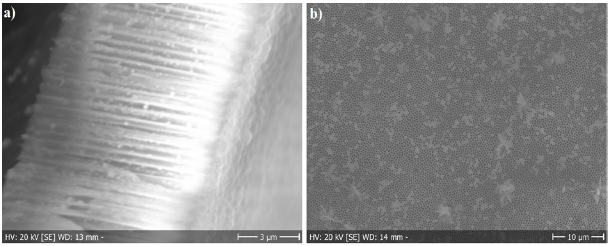

Fig.1 Precursor for Pt deposition a)cross-section b)top.

Obtaining of required electrocatalytically active structures was investigated by two methods: galvanic deposition of Pt and atomic layer deposition of it. For galvanic deposition were variated such parameters as pulse duration (10ms-1s), waiting time and number of cycles (from 100 to 50000). For atomic layer deposition was variated number of cycles from 25 to 200 cycles. As precursors were used $Pt(acac)_2$ and O_3. Both of the methods give the results which were controlled by SEM and EDX-analysis. The objects also were put through its' paces in electrochemical reduction of hydrogen. The representative look of cyclic voltammetry curve is an evidence of the process. Also from cyclic voltammetry data was calculated the amount of deposited platinum.

Further explore will be directed to establishment of mechanism of the process of interaction between AgAu/C nanoparticles with the platinum during both of the types of its deposition. The assumption is that the best catalytical properties will have the structure with AgAu/C nanoparticles covered by platinum because of the highest surface area of platinum particles.

New Electroactive Polimeric Nickel Complex Containing Azogroups

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The technological advances in the last century made obtaining and processing resources much faster and easier, which lead to development and production of new materials. Along with that increased the need in energy production, new ecological and economical problems appeared. The demand for alternative sources of energy grows. Among those are electrochemical current sources.

Polymeric nickel complexes with Schiff bases are promising materials for modification of electrodes for various purposes [1, 2]. These polymers can be used in optoelectronic devices, in detectors, as catalysts in miscellaneous reactions, or they can be used to increase the capacitance of double-layer capacitors [2].

The focus of this research, a polymeric Ni(Ph2N4Salen) complex (Fig. 1), displays an unusual for polymeric salen-type complexes stability in the high positive voltage range. It is also stable in solutions contaminated with water and other electrochemically active species, which allows for increased lifetime of this polymer in energy storage devices.

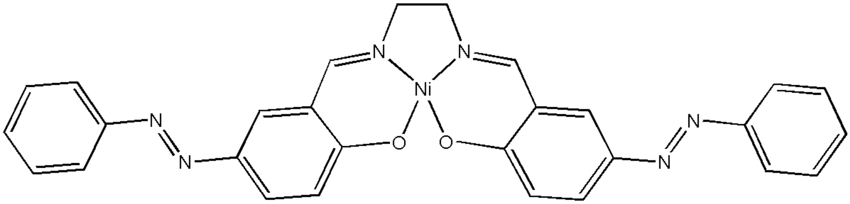

Fig. 1. Ph2N4NiSalen.

Scientific research were performed at the Center for Geo-Environmental Research and Modeling (GEOMODEL), Interdisciplinary Center for Nanotechnology, Center for Chemical Analysis and Materials Research, Center for Thermogravimetric and Calorimetric Research, Center for X-ray Diffraction Methods of Research park of St.Petersburg State University.

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Effect of Electrolyte on Electrochemical Properties of PEDOT/MnO_2 Composite Films

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In recent years, there is a high demand on conducting polymers-based materials, which have such characteristics as high specific capacities and stability. One of the most promising polymers is PEDOT, which composites with transition metals compounds can be used as electrode materials. PEDOT/MnO_2 composites have high specific capacities [1, 2], but there is an uncertainty in its behaviour in different electrolytes.

Herein, we electrochemically synthesized a PEDOT film on the surface of 0.07 cm^2 glassy carbon electrode from 0.1 M acetonitrile/EDOT solution at 0.1 mA/ cm^2 for 100 s. Then, we reduced the film and deposited MnO_2 in PEDOT film by chemical redox reaction from 0.05 M $KMnO_4$ solution for 100 s.

The composite properties were investigated in such electrolytes as 1 M $LiClO_4$/H_2O, 1 M $LiClO_4$/propylene carbonate, $BMIMBF_4$ and $BMIMBPF_6$ ionic liquids by means of cyclic voltammetry, galvanostatic charge-discharge and electrochemical impedance spectroscopy.

PEDOT/MnO_2 composites exhibit different capacities and show significantly different stabilities in these electrolytes. It has also been noticed that there is a "resting effect" on films which results in regaining capacity after leaving films for some time without cycling (Fig. 1).

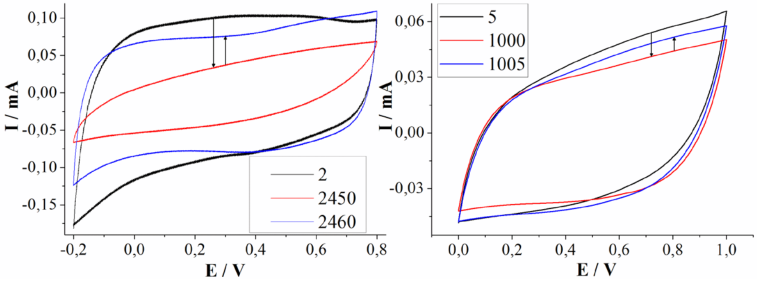

Fig. 1. CVs of PEDOT/MnO_2 in 1 M PC/$LiClO_4$: 2nd, 2450th and 2460th cycles, 72 h between 2450th and 2460th show "resting effect" (left); and in $BMIMPF_6$: 5th, 1000th and 1005th cycles, 1 h between 1000th and 1005th cycles show "resting effect" (right).

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Synthesis, Thermal Stability and Reactivity of Borazine

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Thermal stability and reactivity of borazine was studied in solution and in the gas phase. Borazine $B_3N_3H_6$ was prepared by the reaction between ammonia sulfate and sodium tetrahydroborate in tetraglym at 135°C for 4 hours [1], purified by distillation in vacuum and characterized by IR and NMR-spectroscopy. Vapor pressure of borazine was measured by static tensimetric method [2]. Data in the saturated vapor region are in good agreement with previous studies [3]. In the gas phase borazine slowly decomposes with liberation of molecular hydrogen and formation of polymeric forms.

Reactivity of borazine in deuterobenzene solution in presence of $AlBr_3$ was monitored by NMR spectroscopy. In contrast to B,B',B"-tribromoborazine, which showed fast H/D exchange upon addition $AlBr_3$ in deuterobenzene [4], in case of borazine no H/D exchange was observed. Instead, fast polymerization of borazine with H_2 evolution was evident after addition of $AlBr_3$. The difference can be explained by larger stability of brazonium ion $[B_3N_3H_7]^+$ [5].

Obtained results show that borazine undergoes polycondensation both in the gas phase and in solution, in the latter case decomposition is accelerated by addition of the Lewis acid.

Financial support SPbSU (project № 12.38.255.2014) is gratefully acknowledged. We thank SPbSU Resource Center for Magnetic Resonance for measurements of NMR spectra. Special thanks to Igor Kazakov for help with implementation of this work.

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New Platinum(II) Complexes as Luminescent Probes for Covalent Binding with Proteins

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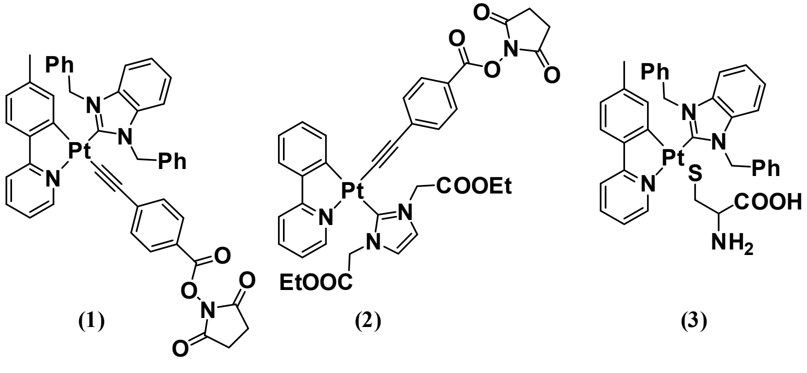
Nowadays the field of luminescent microscopy is attracting considerable attention. Rapidly advancing is the directed synthesis of compounds capable of covalent binding with certain types of biomolecules. A widely used class of probes are transition metal complexes that feature triplet luminescence and bear a fragment designed specifically for labeling biomolecules [1].

Herein we report on the synthesis of three new labels in which the chromophore is a metallacycle formed by a platinum atom and a fragment of 2-phenylpyridine derivate, while *N*-heterocyclic carbenes serve as an auxochromic group. For compounds **1** and **2** functionalized with succinimide esters were obtained conjugates with a co-polymer of vinylpyrrolidone and allylamine [2]. Compound **3** containing a reactive aliphatic amino group afforded an adduct with a C-terminus of a co-polymer of benzyl-L-glutamate and leucine. The photophysical characteristics of free complexes and the respective conjugates have been investigated.



(1) (2) (3)

Fig. 1. New labels for conjugation.

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Complexes of Iridium Based on Dipyridyl Containing Polymers

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Metal-polymer complexes are of interest for optical and photophysical applications [1]. Copolyamides with different contents of dipyridyl groups were obtained by low-temperature polycondensation from 4,4-diamino-2,2-dipyridine, 4,4-diaminodiphenyl ester and dichloranhydride therephthaloyl-bis(3-methoxy-4-oxybenzoic) acid. We obtained metal-polymer complexes with different concentrations of $Ir(ppy)_2$ by interaction of a polymer ligand with dinuclear complexes $[Ir(ppy)_2Cl]_2$ (ppy-2-phenylpyridine) and investigated their properties. Quite efficient luminescence 310a.u. was detected for macromolecular iridium complex, containing 30 mol % bipyridyl units.

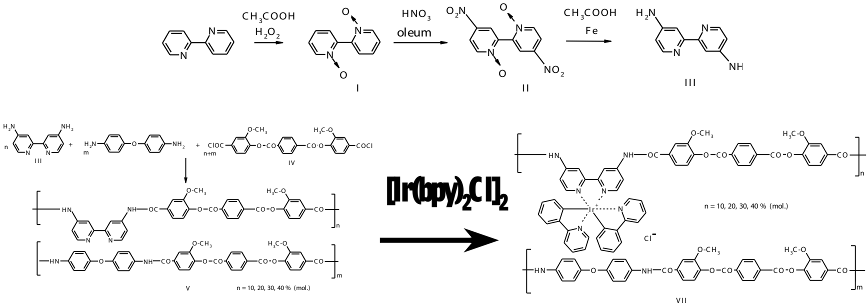

Fig. 1. Scheme of synthesis metal-polymer complex.

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B.Geo- and Astrophysics

Analysis of the Temporal Variability of Methane Concentration in the Atmosphere Near Saint-Petersburg Using *in situ* Observations

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Atmospheric methane belongs to the three major greenhouse gases (H_2O, CO_2, CH_4). According to various estimates, 30% ÷ 60% of the total CH4 emissions are attributed to human activities. Since the industrial revolution mankind has had a significant impact on the concentration of atmospheric methane [1, 2]. Currently, the sources of methane are known with insufficient accuracy, therefore it is not possible with certainty to explain changes of CH4 concentration in the atmosphere, observed in the last decade [1].

The analysis of in situ CH_4 measurements is focused on:

- investigation of temporal variability in the CH_4 concentration for the Peterhof station (SPbU) including irregular disturbances, diurnal and annual cycles of CH_4;
- discussion of the factors influencing the variability of CH_4 concentration;
- comparison of results obtained at the Peterhof station with independent measurements of CH_4 in the atmosphere.

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Revealing Short-Period Normal Modes of the Atmosphere

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The subject of this study is *atmospheric normal modes* (ANMs) [1, 2] in the period range of hours (with periods of ~1 to 5 h). These very weak gravity–inertia ANMs are horizontally two-dimensional Lamb waves. The knowledge about these waves can be useful for investigation of the dynamical processes on the other planets (Mars and Venus).

This work is the first study based on long series of observations originally focused on revealing ANMs in the period range of hours. The core of the study is the search for a periodicity in the frequency distribution of the observed atmospheric oscillations. This periodicity was derived when modeling the spectrum of gravity–inertia ANMs [3].

Barometer and seismometer measurements at Collm, Germany (51.3° N, 13.0° E) for all of 2002 are used to search for atmospheric normal modes (ANMs) in the frequency range 50–310 μHz. The measurements are spectrally analyzed using a 5-day window sliding along the 1-year series with a 1-day step. The subsequent analysis follows two procedures: (a) revealing features in the frequency distribution of the number of statistically significant spectral peaks in histograms built on the basis of these spectra and (b) calculating the multiplication spectra for the raw spectra. The two procedures yield the same result for the two instruments, i.e., reveal a periodicity in the clustering of atmospheric modes on the frequency axis with a period of ~6 μHz. The fact that this period is close to 7 μHz, which is predicted by the crude theory of gravity-inertia ANMs [3] for their frequency distribution, suggests that ANMs are generated down to as small a period as ~1 h.

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Analysis of the Observations of CO_2 Concentration Changes in the Ambient Air at the Peterhof Station for 2013-2014

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Carbon dioxide is one of the most important long-lived greenhouse gases in the Earth atmosphere that increase seems to be one of the reasons of climate changes. CO_2 increase shows the evolution of anthropogenic affection on the biosphere which has been noticed since pre-industrial period, when CO_2 concentrations in the atmosphere have risen by over 30% [1]. This is why ground-based observational networks, aircraft campaigns, satellite experiments with the powerful tools of atmospheric modeling are focused on the investigations of past, present and future of CO_2 in atmosphere [2].

The main targets of the study are as follows:

- to estimate temporal variations of CO_2 concentrations observed at the Peterhof station from 2013 to 2014;
- to compare our results with independent measurements and the modeling results [3];
- to analyze reasons which could be responsible for the variations of CO_2 concentrations;
- to find out how the CO_2 concentration changed for 1 year.

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Hygroscopicity Parameter of Atmospheric Aerosol: Computation from the Cloud Condensation Nuclei Counter Data

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The study of the aerosol particles ability to act as cloud condensation nuclei (CCN) is one of the key objectives of the aerosol climatology, which describes the climatic effect of aerosols. Fine aerosol particles play a crucial role in the formation of clouds. The growth of CCN concentration due to anthropogenic and natural sources leads to increasing the concentration of cloud droplets and decreasing their size that in turn changes clouds lifetime and radiative properties. The CCN properties of aerosol particles depend on their size, structure and chemical composition. At the present time a hygroscopicity parameter is widely used to describe a hygroscopic and CCN behavior of multi-component ambient aerosols [1]. A tandem of Cloud Condensation Nuclei Counter (CCNC-100, DMT) and Scanning Mobility Particle Sizer (SMPS 3936, TSI Inc) was used to measure critical supersaturation for ambient aerosol as function of particles diameter.

The measurements were performed in Saint-Petersburg State University (Petergof) during March – April 2014. The hygroscopicity parameter [1, 2] was computed from the measurement data. This parameter reveals variability and are within 0,1 – 0,9 range because of aerosol chemical composition changes.

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The Relative Humidity Dependence of the Light Scattering by Salt Aerosols

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Aerosol particles play an important role in the transfer of heat and solar radiation in the atmosphere affecting the Earth's radiation budget and thus influencing the weather and climate. The change in the Earth's radiative balance due to aerosol light scattering and absorption is called the direct aerosol radiative forcing. It can be negative or positive, depending on the chemical and microphysical properties of the involved aerosols and the Earth's surface albedo [3].

The optical properties of atmospheric aerosols (scattering and absorption cross sections, single scattering albedo etc.) are highly diverse and strongly dependent on ambient conditions. For example the aerosol light scattering coefficient is influenced by the relative humidity (RH) in the atmosphere. Wet aerosol particles are larger than their dry equivalents, therefore they scatter more light, which has a direct impact on the radiative forcing [1].

To determine the characteristics of the interaction of aerosols with the radiation the particles are mathematically modeled as bodies of certain geometric shape that help in solving the problem of electromagnetic waves diffraction on the aerosols. The simplest case, for which the general solution of the diffraction problem was founded, is light scattering by a homogeneous sphere. This solution is known as Mie theory [2].

This work is devoted to obtaining the RH dependence of the scattering cross section (C_{sca}) of the salt aerosol particles of NaCl and $(NH_4)_2SO_4$.The calculation were made for NaCl and $(NH_4)_2SO_4$ particles in MATLAB environment using "Matlab for Mie" pack. Processing of the data was carried out in the program Origin. The calculated C_{sca} as function of RH is shown in figure. In the RH increasing mode (hydration) humectants make direct phase transition "deliquescence", and in a mode of decreasing RH (dehydration), there is a reverse phase transition "efflorescence". The graph shows that C_{sca} rapidly increases with RH above deliquescence point that indicates a strong effect of high humidity on aerosol scattering in the atmosphere.

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Expansion of the Planetary Disturbing Function in the Computer Algebra System Piranha

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The problem of the expansion of the planetary disturbing function is one of the most important and crucial problems arising in Celestial mechanics. Since the early work of Euler and Lagrange, there have been many suggestions on how to deal with this problem. To date, due to the automatic computation systems, namely specialized computer algebra systems, there has been a significant progress in this direction.

The main goal of this research is to present and implement in the computer algebra system called Piranha an algorithm for the expansion of the planetary disturbing function into the Poisson series using Poincare canonical elliptic elements [1]. These elements allow all intermediate expansions of the Keplerian processor to be expressed as a power series, which makes the disturbing function be also represented as a multivariate power series.

An algorithm for the expansion of the basic intermediate functions of the Keplerian processor into Poisson series is presented [2].

The expansion of the disturbing function is performed up to degree 7 in positional elements and the trigonometric degree 15 in angular elements.

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Statistical Methods of the Separation of Interfering Seismic Waves

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In this paper, we investigate the problem of the separation of interfering seismic waves. The task of separating seismic waves occurs on-example, when working with fields containing many of closely spaced reflective layers or when working with the fields with complex distribution of velocities of seismic waves.

In this work, to solve the problem it was the method of genetic algorithm - a method built on the principles of biological evolution. Since the task is necessary to minimize some of multi function (Fig. 1) optimization analytical methods (such as gradient descent) are not applicable. At the same time the genetic algorithm method shows a good resolution and effectively combats noisy signals.

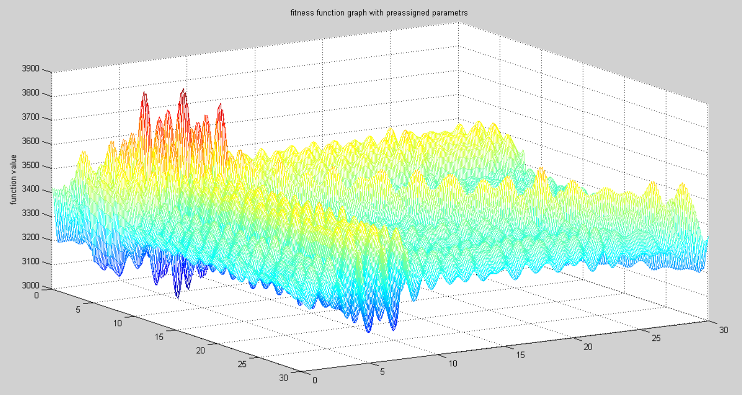

Fig. 1. The function minimized (fitness function).

This demonstrates the accuracy of the genetic algorithm as a function of the difference between the proceeds of signals (in other words, the resolving power), of the dispersion value of noise, that stacks with signals, of the number of the signals and their shapes.

As the aim of this study is to compare the method of genetic algorithm and simulation annealing method. Interestingly, annealing simulation method was also suggested by nature: the optimization method simulates the processes that occur during the cooling of hot metal in the crystal lattice.

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Limb Radiation Vertical Profiles of the Diurnal Martian Atmosphere in the 1.4 and 1.6 mcm Bands of CO_2 as Measured by the SPICAM Spectrometer Onboard the Mars Express Spacecraft

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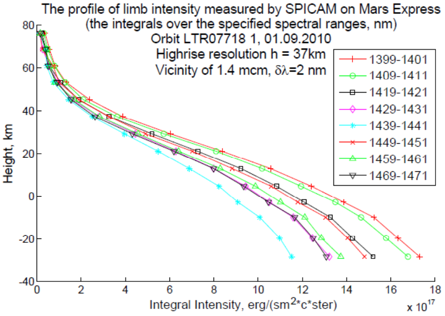
The SPICAM spectrometer developed with the participation of Russian scientists from the Space Research Institute is a multifunctional spectrometer which had been designed for measuring the radiation outcoming from the Martian atmosphere in the ultraviolet (118-320nm) and infrared (1000-1700 nm) spectral channels onboard the Mars Express spacecraft lunched in 2003 year. The instrument is able to detect the radiation with high spectral resolution in different operational modes of observation, including registration of the radiation outcoming from the limb of the planet. For the limb observations, a contribution of the planetary surface to the outgoing radiation is minimized. Therefore, the measurements of the vertical profiles of the limb intensity are potentially the most informative for retrieving both the Martian atmosphere parameters and the optical properties of aerosols permanently presented in it. The spectral measurements of the limb radiation intensity of within the spectral regions of the carbon dioxide 1.4 and 1.6 micron bands are potentially most interesting.

In the present study, the spectra of limb radiation intensity recorded by IR channel of the spectrometer for two orbits (07718 on September 1, 2010 and 02429 on December 3, 2005) corresponding to the minimum of a distance between the spacecraft and the target point have been investigated. Since the aperture of the instrument is equal to 1 degree, for these spectra the best vertical resolution on the limb planet (37 km and 23 km, respectively) has been achieved.

Profiles of the integral intensity depending on the height of the target path along which the outcoming limb radiation is formed, were calculated using the program developed (in C++). Several spectral intervals (with width from 2 up to 50 nm) within the spectral ranges of the 1.4 and 1.6 mcm bands of CO_2 were selected for an analysis.



Using the results of the analysis, some conclusions about an information quantities relative to the problem of retrieving the optical properties of the Martian aerosols were formulated

Magnetic Field of the Sun as a Star and the Sunspot Activity

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A. Severny from Crimea Astrophysical Observatory discovered in 1969 an unusual behavior of magnetic field of the Sun viewed as star [1]. Magnetic field looked as magnetic rotator with significant non-axisymmetric component in the equatorial plane. He tried to relate this field to the sunspot activity but did not find correlations. The origin of magnetic field variations at the Sun viewed as star is still unknown.

In the present work we analyze magnetograms of large-scale magnetic fields observed in Kislovodsk Observatory since 2014 in order to find relations between sunspot and magnetic activity. Results of our analysis demonstrate a contribution of local strong magnetic fields to the mean magnetic field of the Sun viewed as star.

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Estimation of Seismic Waves Parameters with Application of a Genetic Algorithm

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A Genetic algorithm (GA) is an optimization technique that arrives at a solution using a method that simulates the process of evolution in biological systems. GA are very important methods for the solution of non-linear problems. The basic steps in GA are: coding, selection, crossover, mutation and choice. Coding is a way of representing data in binary notation. It is important to be able to record any valid option that could more or less claim to be the solution to the problem. When choosing the number of digits in the parameter note that when a large number of bits improves the accuracy of the solution, but increases the search time of the decision. To encode any parameter can seismic waves, for example, velocity. The algorithm must now determine the fitness of the individual models. This means that the binary information is decoded into the physical model parameters and the forward problem is solved. The resulting synthetic data is estimated, then compared with the actual observed data using the specific fitness criteria. Next step is selection. The selection of pairs of the individual models for the reproduction is based on their fitness values. Models with the higher fitness values are more likely to get the selection than models with low fitness values. A crossover caused the exchange of some information between the paired models thereby generating new models. The last genetic operation is a mutation. The mutation is a random change of binary state. The condition of the procedure of mutation: if a value obtained by a random number generator is less than a certain threshold value, the mutation procedure is performed. The last basic step in GA is choice. We choose from each pairs a model, which has the less fitness function. Then we produce the procedures: the crossover, the mutation and the choice. This procedure is continued until we obtain the optimal model.

In this paper we have used the GA for the estimation of the velocity for the gradient layer. The synthetic seismogram was calculated by the finite-difference method. The obtained results showed higher effectiveness GA for the velocity estimation.

C. Mathematics and Mechanics

Stable Periodic Solutions of Generalized Logistic Equation with State-Dependent Delay

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Logistic equation with delay plays important role in population dynamics. In this work we consider its generalized form:

$$\dot{N} = \lambda N\left[1 - N\left(t - T\left(N\right)\right)\right], \qquad (1)$$

$\lambda > 0$ is a parameter. We suppose $T(N)$ is analytical function, $T(1)=1$ and $0<T(N)<T_1$, for some positive T_1. Decomposition of $T(N)$ in Taylor series is

$$T(N) = 1 - \alpha(N-1) - \beta(N-1)^2 + o((N-1)^2),$$

where α, β are nonzero parameters. Also we suppose all the considered solutions of equation (1) are bounded.

The problem is to research local dynamics of equation (1) near the equilibrium $N_+ = 1$ and also to study its some nonlocal properties. It is well known if $\lambda < \pi/2$, this equilibrium is asymptotically stable, and if $\lambda > \pi/2$, it is unstable. So we assume $\lambda = \pi(1+\varepsilon)/2$, where ε is small positive parameter.

In the first part of this work we research Andronov – Hopf bifurcation, which occurs in (1) near N_+. Namely, we obtain simple sufficient condition that equation (1) has stable periodic solution in sufficiently small neighborhood of equilibrium N_+. This condition is:

$$(\alpha,\beta) \in \left\{(x,y) \in R^2 | \beta_0 < y,\ \alpha_-(\beta) < x < \alpha_+(\beta)\right\},$$

$$\beta_0 = \frac{9(\pi-4)(3\pi-2) - 32(1+\pi)^2}{135\pi(4-\pi)},$$

$$\alpha_\pm(\beta) = \frac{16(1+\pi) \pm 2\sqrt{270\pi(4-\pi)(\beta-\beta_0)}}{9\pi(4-\pi)}.$$

For this purpose we use asymptotic method of normal forms. Using this method we also construct an asymptotic approximation of detected periodic solution.

In the second part of the work we research the situation when sufficient condition of Andronov – Hopf bifurcation if not met. In this case equation (1) may have periodic solutions, for which relaxation oscillations correspond.

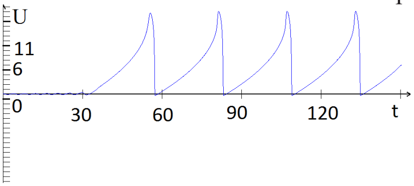

Fig. 1. Graph of solution of (1) when $\alpha = -3$, $\beta = 0.1$, $\varepsilon = 0.01$.

Dynamics of Mapping and Stable Regimes of Singulary Perturbed Neuron System

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Let us consider a chain of diffused connected and singularly perturbed nonlinear differential equations with a delay:

$$\dot{u}_j = d\left(u_{j+1} - 2u_j + u_{j-1}\right) + \lambda\left[-1 + \alpha f\left(u_j\left(t-1\right)\right) - \beta g\left(u_j\right)\right]u_j, j = \overline{1,m} \qquad (1)$$

where $m \geq 2, \lambda >> 1, \beta > 0, \alpha > 1+\beta,\ u_j > 0, u_0 = u_1, u_m = u_{m+1}$. The smooth functions $f(u), g(u) \in C^2(R_+)$ have entry conditions:

$$f\left(0\right) = g\left(0\right) = 1,\ 0 < \beta g\left(u\right) + 1 < \alpha,\ \forall u \in \mathbb{R}_+;$$

$$f\left(u\right), g\left(u\right), uf'\left(u\right), ug'(u) = O(1/u),\ u \to +\infty.$$

In articles [1,2] there was made a transformation of system (1) to the system of differential equations with impulsive influences. Let us consider a mapping:

$$\Phi\left(z\right): \begin{pmatrix} z_1 \\ \vdots \\ z_{m-1} \end{pmatrix} \to \begin{pmatrix} y_1(T_0) \\ \vdots \\ y_{m-1}(T_0) \end{pmatrix}, \qquad (2)$$

where the functions y_j are connected with initial variables by means of asymptotic equations $y_j \approx \ln u_{j+1} - \ln u_j$. $(y_1(t), \ldots, y_{m-1}(t))^T$ is a solution, where $y_1\left(-0\right) = z_1, \ldots, y_{m-1}\left(-0\right) = z_{m-1}$. $T_0 = \alpha + 1 + (\beta+1)/(\alpha-\beta-1)$ is the first approximation of stable cycle of single oscillator of system (1).

In articles [1, 2] there was proved a statement that exponential stable points of mapping (2) are satisfied the orbital asymptotic stable cycles of system (1). An asymptotic analysis of mapping (2) shows that it has at least n+1 stable points and zero point is stable for any values of *d*.

As the result of numerical research there were found different stable regimes of dynamic system. These results coincide with the results of theoretical asymptotic form. Also there were found the cases of coexistence of greater number of stable points. In the article [3] there were considered reconstructions of phase portraits for cases of 5 and 7 stable points for two-dimensional mapping (2).

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Precipitation Regions in the Problem of Charged Particles Dynamics in the Earth's Magnetic Field

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The motion of a charged particle in the earth's magnetic field has long been of long interest to mathematicians and physicists in connection with the study of the polar aurora and cosmic rays. The mathematical formulation of this problem was given by Stormer as early as 1907, it is often referred to as Stormer's problem.

We consider the approximation of the Earth's magnetic field. For different models we calculate the number of charged particles trajectories which intersect the Earth's surface. The precipitation regions is the region in plane that corresponds to angular spherical coordinates of the final point where the particle under consideration falls to the Earth. Influence of kinetic energy on such region is investigated in the paper.

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Circle and Popov Criteria for the Systems with Multiple Nonlinearities

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Absolute stability for nonlinear systems plays an important role in the history of automatic control theory. An important event in the late 1950s and early 1960s was discovery of the frequency-domain absolute stability criterion by the V.M. Popov [1]. Though original Popov's proof did not rely on the Lyapunov functions it has become clear soon that fulfillment of the Popov's frequency-domain condition is sufficient for existence of Lyapunov function from the class ”quadratic form of the system state variables plus integral of nonlinearity”. In 1964 V.A. Yakubovich has proven [2] that in the case of one nonlinearity the Popov's frequency-domain condition is necessary and sufficient for existence of Lyapunov function. Analogous result for the circle criterion and quadratic Lyapunov function was obtained in [3].

Both circle criterion and Popov criterion were soon extended to the systems with several nonlinearities (MIMO case). However equivalence of those criteria to existence of appropriate quadratic Lyapunov functions was not established until recently. The main reason is, perhaps, in that the losslessness of the S−procedure (S−theorem) for several quadratic constraints in general does not hold.

In this paper the equivalence between circle and Popov criteria and the existence of corresponding Lyapunov functions for MIMO Lurie systems is established for the case when each sectorial constraint defines an infinite sector. In such a case S−theorem holds for any number of constraints and this fact is used in the proof.

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Synchronization in Heterogeneous FitzHugh-Nagumo Networks

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Synchronization in neural networks has gained a lot of attention lately since it is involved in processes as diverse as learning and visual perception on the one hand and the occurrence of Parkinson's disease and epilepsy on the other hand. Study of synchronization has so far focused on networks of identical nodes. However, in realistic networks the nodes will always be characterized by some diversity meaning that the parameters of the different nodes are not identical but drawn from a distribution. It is well known that such heterogeneities in the nodes can hinder or prevent synchronization and that the coupling strength is a crucial parameter in this context.

In this work we study synchronization in networks of heterogeneous FitzHugh-Nagumo nodes [1, 2], a generic model for neural dynamics. We find the condition of synchronization in this network and offer the algorithm to control it in the case of synchronization absence. The simulation results confirm the efficiency of proposed control method.

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Comparison of the Monte Carlo Method for Solving Stochastic Differential Equations with Some Existing Numerical Schemes: Euler-Maruyama Method and Milstein Method

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In this report the family of Monte Carlo methods for solving stochastic differential equations is introduced. They share the same two-step approach: transformation of differential equation into an integral equation and implementation of Neumann-Ulam scheme [1-5].

The existing numerical schemes for solving stochastic differential equations have well-known methods for solving differential equations as their basis – the Euler-Maruyama method, the Milstein method and the family of Runge-Kutta methods [6]. They provide an approximate solution that has both random and systematic error.

The original methods considered in this report don't have a systematic error in a lot of cases.

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Takens Method for Nonholonomic Systems

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Takens method is a group of approaches to the analysis of time series generated by nonlinear deterministic dynamical systems. It typically allows us to reconstruct an unknown dynamical system that gives rise to a given observed scalar time series simply by constructing a new state space out of successive values of the time series. This provides the theoretical foundation for many popular techniques, including those for the measurement of fractal dimension and Lyapunov exponents [1].

Application of this method to the nonholonomic systems on sub-Riemannian manifold is considered. This systems occur in a great variety of problems e.g. robotics and industry [2].

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D. Solid State Physics

Low Temperature Optic Investigation of CdMgTe/CdTe Heterostructures with Ultrathin MnTe Layers

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The influence of ultra thin layers on the properties of nanostructured materials is an important problem for science and technology. The special interest is the incorporation of magnetic layers due to the possibility affect strongly on the properties of heterostructure by means of an external magnetic field.

In our work the CdMgTe/CdTe heterostructures with ultrathin MnTe layers were studied. A schematic diagrams of electron energy profiles for samples under consideration are presented in Fig. 1.

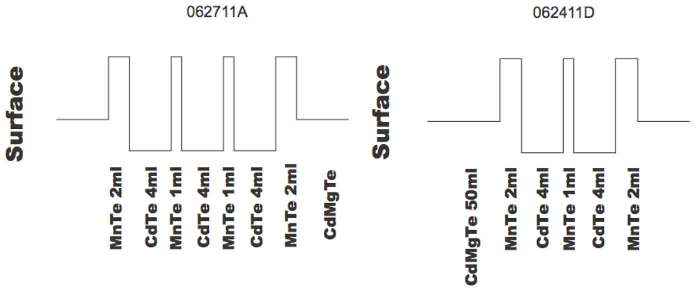

Fig. 1 A schematic diagrams of electron energy profiles of the analyzed samples.

The comparison between the luminescence and the reflection spectra enables us characterize the luminescence structure as the emission of barrier and quantum well excitons (Figs. 2 and 3).

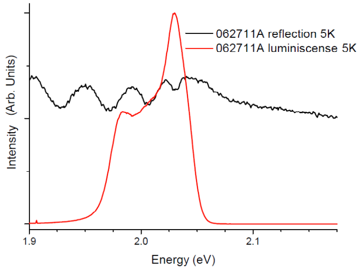

Fig. 2 Spectra of Reflection and Fotoluminiscense of sample 062711A.

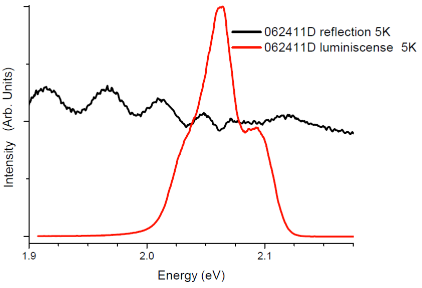

Fig. 3 Spectra of Reflection and Fotoluminiscense of sample 062411D.

The structure of luminescence spectra and its temperature dependence is also discussed.

Influence of the Surface Localized Plasmon Resonance in Gold Nanoparticles on the Photochemical Activity of Titanium Dioxide

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Titanium dioxide is widely used in industry due to its semiconductor properties. It is used for preparations of self-cleaning surfaces, the water and air treatment systems, and in system for the water splitting. But titanium dioxide has a wide band gap. Therefore, the fundamental absorption is in the UV spectral region. One of the way for sensibilization of titanium dioxide to visible light is the effect of the surface localized plasmon resonance [1].

Here TiO_2 samples with different structures namely thin film of titanium dioxide with gold nanoparticles were synthesized and explored their surfaces by SEM to determine the size of the nanoparticles. Samples were characterized by XRD, absorbtion spectroscopy. The spectral dependence of the photocurrent (Fig. 1) was measured. It was found that photocurrent under irradiation by visible light was several times higher for samples with gold nanoparticles than pure samples. The change in work function upon irradiation by visible and UV light was explore using Kelvin Probe and analyzed.

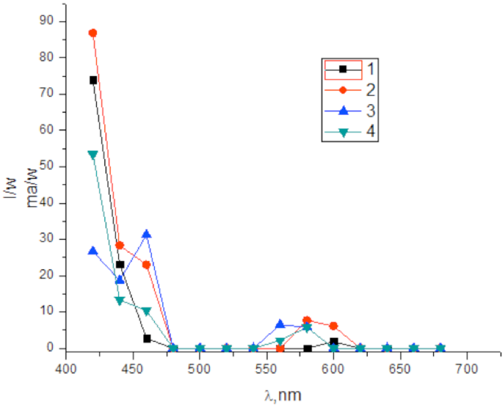

Fig. ***1.*** *1 – TiO_2 (black), 2 – Au-TiO_2 (red), 3 – TiO_2–Au–TiO_2 (blue), 4 – N-TiO_2–Au–TiO_2 (green).*

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Acoustic Studies of Ferroelastic Phase Transition in $LiCsSO_4$ Nanoparticles Embedded in the Pores of MCM-41 Molecular Sieves

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Studies of influence of size effects and confined geometry conditions on phase transitions (PT) of different nature is important both for fundamental and applied physics. The ferroelastic PT is one of the least studied types of structural phase transitions. Direct information about changes of the structure at this type of PT can be obtained via measurements of the temperature dependence of an elastic modulus conjugate to the order parameter. Most complete data in such kind of studies can by obtained by acoustic methods which are actively used in the case of bulk ferroelastics [1, 2].

Up to now there is only one paper devoted to the ferroelastic PT in nanoparticles [3]. The paper presents results of the measurements of the temperature dependence of a shear ultrasound velocity in a nanocomposite on the base of molecular sieves MCM-41 with ferroelastic $LiCsSO_4$ nanoparticles in the pores.

In this report we present the results of a similar study for the MCM-41/$LiCsSO_4$ nanocomposite but, in contrast to [2], with use of the longitudinal acoustic wave. The measurements were carried out at a wide temperature range including the temperature (202 K) of the ferroelastic PT from the paraphase (mmm) to the ferroelastic one (2/m) at the bulk crystal. The primary (microscopic) order parameter is linearly coupled with the component ε_{xy} of the strain tensor. The obtained results are compared with the data of the paper [3]. In contrast to the bulk crystal, a sufficiently high sensitivity of the longitudinal wave velocity to this PT in the nanocomposite was observed. A model to explain this phenomenon is proposed.

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Single-Ion Anisotropy Influence on the Magnetic Ordering in RMn_2O_5 Compounds Under Rare Earth Substitution

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Magnetic multiferroics where the ferroelectricity develops at the magnetic ordering are the subject of significant consideration in the recent years. Their appeal is stemming from a large number of evidences of the correlation between magnetic and electrical properties, which is hopeful for potential applications in functional devices.

The rare earth manganites family RMn_2O_5 attracts the particular attention since these compounds demonstrate the most impressive examples of coupling between magnetic and electrical properties. A large amount of magnetoelectric effects was found in RMn_2O_5.

The evolution of multiferroic $Nd_{0.8}Tb_{0.2}Mn_2O_5$ magnetic structure was studied by means of polarized neutron diffraction. It is shown that doping of the parent compound $NdMn_2O_5$ with terbium leads to noticeable changes in the structure of the magnetic interactions. As in $NdMn_2O_5$, in the system $Nd_{0.8}Tb_{0.2}Mn_2O_5$ there are two incommensurate magnetic phases in a wide temperature range. However, the features single-ion anisotropy Tb^{3+} lead to disproportionate ordering the magnetic moments of Mn^{3+} in the direction of *a*.

The results of research methods polarized neutron scattering show that in the magnetic structures of single crystal $Nd_{0.8}Tb_{0.2}Mn_2O_5$ there is a difference in the population of domains with the "right" and "left" spirals.

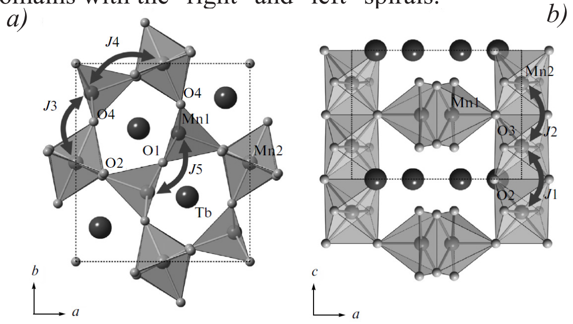

Fig. 1. Crystal structure of RMn_2O_5: projections on the (a) ***ab*** *and (b)* ***ac*** *planes are shown.*

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Effect of Titanium Substitution on the Fe Coordination Sites in the $Sr(Fe,Ti)O_{3-\delta}$ Structure Depending on Ti Content

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Nowadays fuel cells are considered as a promising alternative to the traditional sources of the energy. Currently, one of the critical targets for the development of SOFC is lowering the operation temperature. Reducing the working temperature (from 1000°C to 500°–800°C) will obviously widen the material selection, minimize the interactions between the electrode and electrolyte and reduce the cost. Also in the last few years there has been a growing interest in the research of potential symmetrical electrode materials for SOFC application. The fuel cells of such configuration will allow overcoming two serious drawbacks of SOFC-technology: carbon deposition and sulphur poisoning.

The perovskites based on the $SrFeO_{3-\delta}$ with high mixed electronic and ionic conductivity are very promising candidates from both points of view. However, at intermediate temperature the $SrFeO_{3-\delta}$ undergoes transition into brownmillerite-type structure (SrFeO2.5), in which the oxygen vacancies are ordering. Such transition is not favorable for SOFC operation because the oxygen transport rates are reduced when the vacancies are locked in the tetrahedral layers of SrFeO2.5. Also the decomposition of the cubic phase SrFeO3-δ may cause a volume change of the anode during the oxidation and reduction cycles, causing the splitting of the cell layers. One of the ways to solve the problem of cubic phase stabilization of $SrFeO_{3-\delta}$ is incorporation of high valence transition metals in Fe site cations positions. The partial substitution of Ti atoms for Fe site cations produces a smaller change of the unit volume cell compared to the parent compound $SrFeO_{3-\delta}$ that allows retaining high levels of electronic and ionic conductivity.

The current work is directed to investigation of the effect of Ti substitution on the Fe sites coordination in the $Sr(Fe,Ti)O_{3-\delta}$ structure depending on the Ti content. It was established the change in the formal oxidation state and symmetry of the coordination of Fe-sites cations at Ti concentration higher than 10%. The possible reasons for this fact are: 1) lowering the oxidation of iron from Fe^{4+} to Fe^{3+}; 2) distortion of octahedral environment of Fe; 3) changing the proportion of the tetrahedral and octahedral coordinations of Fe atoms depending on the content of Ti. One can presume that stabilization of the cubic structure $SrFe_{1-x}Ti_xO_{3-\delta}$ is possible only at small concentration of titanium (less than 10%).

Ferromagnetic Ordering of Mn/Si and $Mn_{1-x}C_x$/Si Interfaces

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Formation of magnetic films on semiconductors surfaces are of great fundamental and technological interest because they are very promising for spintronic devices. Especially much attention was paid to the magnetic semiconductors and to the silicides of transition metals, in particularly manganese silicides, which can be integrated into the standard silicon-based technology. Despite the fact, that there is no any bulk Mn-Si phases with a Curie temperature above 50 K, ferromagnetism near and above room temperature was observed in thin Mn/Si structures. One of the possible reasons is the presence of carbon in the grown manganese silicide film, which can results in anisotropic modification of the local structure around the Mn sites. The aim of the present work was to study the role of carbon doping in high-temperature ferromagnetism of Mn/Si interface.

The experiments were carried out in ultrahigh vacuum (10^{-10} mbar) using the Russian–German beamline of the synchrotron radiation at the HZB Bessy II electron storage ring. We have investigated the initial growth (up to 2 nm) of both pure and carbon-doped manganese films on Si(100)2x1 surface. Manganese films were deposited on the silicon substrates from a thoroughly degassed source. Their carbon doping was carried by the use of C_3H_6 adsorption during Mn deposition. The elemental and chemical compositions of the films were studied by high-resolution photoelectron spectroscopy while the magnetic properties were analyzed by magnetic linear dichroism in Mn 3p core-level photoemission.

It has been shown that the manganese deposition on Si(100)2x1 surface with and without carbon doping results in the formation of the interfacial MnSi silicide and the solid solution of silicon in manganese. The Mn film covered with segregated Si begins to grow on the samples surface at coverage of 9 Å of Mn. The main difference between two systems is reduction of segregated silicon on the sample surface in carbon-doped system. The high-temperature ferromagnetic ordering arises in both systems at the coverage of 2-4 Å of Mn. The magnetic asymmetry amplitude of the MLD effect is equal to 3 and 2.2% for carbon-doped and undoped films correspondingly that demonstrates essential influence of carbon on magnetic properties of the films.

The study was supported by Russian Foundation for Basic Research (Project no. 13-02-00398) and the Russian-German Laboratory at HZB-BESSY.

Rates of Magnetic Transitions Controlled by the Exchange Interaction on Atomic Scale

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Magnetization reversal process of a 3d-cluster on the tip apex of an atomic force microscope (AFM) [1] is investigated on the basis of transition state theory for magnetic degrees of freedom. The multidimensional energy surface as function of the angles which determine the orientation of all magnetic moments of the system has been calculated within the framework of the non-collinear Alexander-Anderson model. The energy of the ground and metastable states coincide well with the results of density functional theory [2]. Minimum energy paths on the energy surface determined by the Geodesic Nudged Elastic Band method [3] determine the energy barriers between states as shown in Fig. 1. The rate of magnetic transition is proved to be determined by the exchange interaction between atoms of the cluster on the tip apex and a magnetic sample. The results of our calculations reproduce the lifetime of magnetic states measured by Magnetic Exchange Force Microscopy [1].

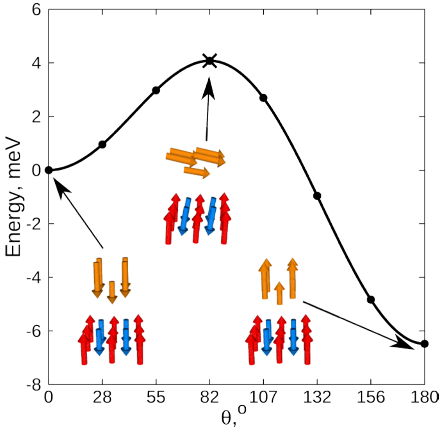

Fig. 1. Energy along the minimum energy path as function of angle between magnetic moment of the foremost atom of the tip and easy axis of anisotropy.

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Photoluminescence of CdSe/ZnS (Core/Shell) Quantum Dots on an Array of GaAs Nanowires

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Semiconductor quantum dots (QDs) A^2B^6 (CdS, CdSe, CdTe) generate the tremendous interest in the field of physics, chemistry and engineering [1-2]. They represent a class of quasi-zero-dimensional objects in which the quantum size effect the energy spectrum occurs due to the spatial limitation of the charge carriers and excitons in all three spatial dimensions.

Methods of colloid chemistry of QDs synthesis extensively used today enable to receive nanocrystals with the size of 1-10 nm in organic solvents. To prevent aggregation of QDs surface-active substance - trioctylphosphine oxide (TOPO) is used [1-2].

At the centre of interest in A^2B^6 QDs are their optical properties: the high quantum yield of photoluminescence (PL) and photostability, the wide absorption spectrum range and narrow band of the PL, the dependence of emission wavelength on the QD size. The possibility of the existence of QDs in the form of colloidal solutions allows to introduce them on developed surfaces that extend the possibility of composite materials creation [1].

In present work we use colloidal CdSe/ZnS (Core/Shell) QDs, deposited on the surface of CdSe nanocrystals and an array of GaAs nanowires (NWs). ZnS «shell», formed around CdSe «core», as a passivator of surface states and as localizer of electron-hole pairs in the nucleus increases significantly the quantum yield of PL [1]. The morphology of the samples was studied by electron scanning microscopy. We investigated the photoluminescence of the samples at $T = 293^o$ K and different atmospheric pressure. Quantum-shift was determined from the luminescence spectra of QDs on the surface of single-crystal CdSe, this allowed to define size of the QDs (~5 nm). The character changes PL of QDs with time was obtained at atmospheric pressure and vacuum. Impact of recharging the surface states due to the adsorption/desorption H_2O and O_2 molecules on the PL kinetics of QDs is discussed. The results suggest a promising use of NW+QD systems in optoelectronics.

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Melting and Crystallization of an Indium-Gallium Alloy Embedded into Porous Glass

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Studies of the melting and crystallization phase transitions for materials under confined geometry conditions are interesting both for fundamental physics and for applications in the modern technology [1, 2].

The present report is devoted to acoustic studies of nanocomposites on the basis of porous glass with average pore size of 7 nm filled with the indium-gallium alloy (9 at.% In, 91 at.% Ga). The indium-gallium alloy was embedded into the pores under pressure of about 9 kbar. Measurements were performed by pulse-phase technique [3] using longitudinal acoustic waves with frequencies 7 MHz. At that signals from two acoustic pulses – reflected from front face of the sample and passed one time through the sample – were compared. The Apiezon N grease was used for acoustic contact between the sample and acoustic duct.

Temperature dependencies of the ultrasound velocity were measured in the temperature range 140-315 K at complete cooling-heating cycles. Ordinary thermal hysteresis loop was observed. The average melting temperature was equal to 269 K that implies the formation of α-gallium on freezing. The shift of the melting temperature range of the alloy in the nanopores relative to the bulk is interpreted in the frameworks of a thermodynamic model based on the Gibbs–Thomson equation.

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Photoinduced Hydrophilic Conversion of Hydrated ZnO Surface

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The effect of photoinduced superhydrophilicity is widely investigated because of its great practical importance since it was discovered in 1997. It is applied for the creating of self-cleaning and anti-fogging glass, self-cleaning coating for exterior and interior surfaces for buildings, tunnels and so on.

The exploration of the influence of various factors on surface hydrophilicity is important task to understand the nature of the photoinduced hydrophilicity phenomenon and to manage the hydrophilic properties of the surface. In this work, the effect of the surface acidity on photoinduced hydrophilicity of ZnO thin films was investigated. ZnO was chosen as a material for the study because of its physical and chemical properties. This semiconductor has a bandgap of about 3.4 eV, it is not expensive and photoactive in the visible spectral region.

ZnO films were synthesized with sol-gel method from zinc acetate dihydrate. The three-step procedure was used to have the initial state of the ZnO surface free of organics and control the conditions during the water wetting and the irradiation steps. The kinetics of photoinduced hydrophilic conversions for ZnO films were obtained and demonstrated the dependence on initial hydrophilic state.

The results are following:

Hydrophilic properties of ZnO surface after treatment in the solution depend on the acidity of this solution. The higher surface acidity (the lower pH value) leads to the lower surface hydrophilicity (the higher water contact angle). There is no conversion into the superhydrophilic for ZnO nano-films independently of the surface acidity. The multi-layered model of hydroxyl-hydrated coverage of the surface is proposed to explain the experimental results.

The mechanism of photoinduced hydrophilic conversion is suggested and includes the generation and trapping of photoinduced charge carriers at the surface defects or photoexcitation of the surface states, which is changed the structure of the hydroxyl-hydrated multi-layer. Spectral study showed the different effect of irradiation on the ZnO surface hydrophilicity: “slow” transformation in the case of fundamental absorption of zinc oxide and “fast” hydrophilic alteration for extrinsic photoexcitation.

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Spin Relaxation Length in Palladium Thin Films

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The development of spintronics (the field of science that examines the behavior of systems, based not only on charge transfer, but on magnetic properties of nano-objects as well) requires study of various magnetic and electrical properties of nanoscale systems. One of the areas of research is connected with study of how efficiently polarized electrons pass through different solid state structures. Number of electrons that passed a certain distance without scattering is determined by inelastic mean free path and is well studied. But important and not sufficiently studied part of transport is connected to spin relaxation. From literature it is known that palladium can, due to its electronic structure, be used for creating solid state spin detectors [1].

In this study we measured lengths of spin relaxation in palladium. The basic idea behind the experiment is to measure polarization of secondary electrons emerging through the Pd. Measurements were conducted as follows: thin films of Pd were deposited on a ferromagnetic single crystal, for each thickness of the film the polarization of the electrons, passed through film was measured for different electron energies. Results of experiment were used for creation of a map of spin relaxation lengths in palladium for various energies and thicknesses.

Preliminary results say about the unique spin properties of palladium films and characterize it as a promising material for spintronics. For instance, we anticipate that palladium can not only be used in electron spin detectors, but can play a significant role in spin-polarized positron experiments [2].

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Atomic Structure and Electronic Properties of Chemically Doped Graphene on Metallic Substrates

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One of the most suitable ways of tuning the electronic properties of graphene for applications in nanoelectronics is chemical doping with nitrogen [1, 2] and boron [3, 4] atoms. In case of epitaxial growth of graphene on metallic substrates, doping can be implemented by a chemical vapor deposition (CVD) method from the gaseous dopant-containing precursor.

As it was demonstrated previously [5], incorporations of the dopant atoms can lead to appearance of several kinds of bonds between impurities and carbon atoms into the graphene matrix. Each of these configurations has a strong effect on the electronic structure of the system.

Investigations were performed at the Resource Center "Physical Methods of Surface Investigation" (RC PMSI) of Research park of Saint Petersburg State University. The work was supported by RFBR (Grant 14-02-31150) and Saint-Petersburg State University

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Impact of AlN Layer Thickness on Their Microstructure and Electric Properties on Silicon

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Aluminum nitride is a wide gap semiconductor that is considered as a perspective material for many applications. Of particular interest is the usage of AlN as a high-k dielectric in silicon-based metal-insulator-semiconductor (MIS) structures [1, 2].

The most of the published papers were devoted to investigations of the crystal structure of AlN thin films obtained by diverse growth technique (for review see [1]) while the information about their electrical properties is scant. In this report the for first time results of the investigation of electric properties of AlN layers on silicon as a function on their thickness are presented.

Au-AlN-Si structure were obtained by reactive magnetron sputtering of aluminum in nitrogen-containing ambient onto silicon substrate following by thermal evaporation of gold. According to scanning and transmission electron microscopy data the obtained AlN films exhibited nanocrystalline granular structure with the hexagonal structure of the grains. The average grain size increases with film thickness increase reaching a value of about 10 nm for the thickest 130 nm film.

The obtained MIS structures were investigated with capacitance-voltage (CV), current-voltage (IV) and deep level spectroscopy (DLTS) techniques.

An analysis of the obtained measurement results revealed the presence of the electronic traps at the AlN-Si interface and in the bulk of AlN layers. The density of the interface states was found of the order 10^{10} cm^{-2} regardless of thickness of the films.

The density of the bulk traps and the film resistivity decreases with the AlN layer increase. They were as high as $10^{19}cm^{-3}$ and $3*10^{11}$ Ohm*cm for 5 nm AlN film while only $10^{16}cm^{-3}$ and $7*10^{9}$ Ohm*cm for 130 nm film respectively.

Bearing in mind the results of the microstructural investigations the described behavior of electric properties can be explained when the bulk traps are situated at the boundaries of the grains of AlN films. The nature of these traps is still not exactly known. Nitrogen vacancies or oxygen impurity are suggested to be possible candidates.

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The Interaction of Topological Insulators Bi_2Se_3 and $Bi_2Te_{2.4}Se_{0.6}$ with Deposited Thin Ni Layer

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Topological insulators (TIs) are new widely studied materials. In contrast to ordinary insulators, the bulk band gap of a TI owes its existence to band inversion and strong spin-orbit coupling. Its surface is metallic due to spin-polarized surface states where the spin is such that surface-state electrons that propagate in opposite directions carry opposite spins. This chirality is caused by time-reversal symmetry, and it prevents electron backscattering. The surface state itself and the topology of its band dispersion E(k) are protected against distortions such as surface impurities by time-reversal symmetry.

The second generation of three-dimensional TIs, such as Bi_2Se_3 and Bi_2Te_3, forms simple systems, with the topological surface state appearing as a single Dirac cone at the Γ point of the surface Brillouin zone. The band gaps are large enough to allow for room-temperature applications, but as-grown samples show a tendency for defects, such as Se vacancies and antisite defects, which lead to an n-type bulk doping (electron doping) so large that the samples are rendered metallic in their bulk. The interaction between three-dimensional TI and doped magnetic impurities can modify the electronic and magnetic properties of the TI, and the results may strongly depend on the types of magnetic atoms, occupation sites of the magnetic impurities, and experimental conditions under which they are introduced. For example, doping Fe and Cr into the bulk Bi_2Se_3 crystal or thin film during the growth process [1, 2] leads to a gap opening at the Dirac point.

This work is devoted to the investigation of interaction between Bi_2Se_3 and $Bi_2Te_{2.4}Se_{0.6}$ TIs with a Ni layer deposited atop. The experiments were carried out at Resource Center “Physical methods of surface investigation” of St. Petersburg State University and at MAX-Lab synchrotron (Lund, Sweden). Electronic structure of the samples was studied by XPS and ARPES methods. It was established that upon Ni deposition, additional components appear in Bi and Se core levels. And the heating of the sample leads to significant changes in its valence band electronic structure.

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Shape Resonances and PEVE Correlations in the Inner-Shell Photoemission from the Molecule CO and the Solid

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The interaction of photoelectrons with the valence electrons (PEVE correlation) is reviewed in the framework of the quasi-atomic model of photoprocesses in polyatomic compounds [1]. The main attention is paid to the influence of the PEVE-correlations on the contour of the shape resonances near the *1s* ionization threshold of carbon atom in the Σ photoionization channel of the molecule CO and the solid. The advance of the quasi-atomic approach, the concepts of the potential barrier and the optical potential are used. The $(M_\Gamma{*}L{*}G)(k)$– function method applied to describe the intramolecular interference of the primary photoelectron with elastically scattered photoelectron waves. It is found that doubly excited states

$$C\ 1s^{-1}\,5\sigma^{-1}\,2\pi^{2}Ryd^{1}\ (\mathrm{S}=1) \text{ and } C\ 1s^{-1}\,1\pi^{-1}\,2\pi^{2}$$

play the most important role in forming the contour of the shape resonances in the molecule CO. It is predicted that the state $C\ 1s^{-1}\,1\pi^{-1}\,2\pi^{2}$ leads to the ultrafast dissociation of the molecule [2]. For the first time the cross section of inelastic scattering of the photoelectron on valence electrons in the ionized molecule near the *C 1s* threshold is determined. It is shown that the state $C\ 1s^{-1}\,1\pi^{-1}\,2\pi^{2}$ dominates in the *C 1s* photoemission from the CO-solid. This work is supported by the Saint-Petersburg State University grant # 11.38.638.2013.

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Photoelectron Study of the Interface in Si/TiN/IL/HfO$_2$ Structures with Different Interlayers (IL)

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Nowadays the size of the critical parts of microelectronic devices had already reached to the range of few nanometers. Analysis of different metal – insulator-metal (semiconductor) structures reveals that the interlayers (their extension and composition) generated at the metal/insulator interfaces owing to processes such as interdiffusion and chemical reactions can play an important role. For example, the interlayers can influence on the energy barrier for electrons at the interface and as a result can change the effective work function. The problem can be solved by inserting of thin interlayers at metal/isolator interface.

This work is directed to the investigation of Si/TiN/HfO$_2$ structure with focusing on the formation of the interface with/without thin interlayer assembled between HfO$_2$ film and TiN electrode. The TiN/HfO$_2$ entity has a wide application in advanced logic and memory semiconductor devices [1] and is of great interest.

The researches were carried out using X-ray photoelectron spectroscopy of high kinetic energies (HAXPES). Due to a large value of inelastic mean free path, HAXPES is a very effective non-destructive depth sensitivity technique for chemical analysis of nano-layered systems. In the current work the depth profiling of the samples was realized by changing the photoelectron's emission angle at fixed exiting photon energy. It was established:

- Due to the oxygen scavenging the oxidation of TiN electrode occurs in the system HfO$_2$/TiN.
- The insertion of Al$_2$O$_3$ thin layer restricts to some extent the interdiffusion in this system.
- The inserted TiO$_2$ thin layer reacts actively with TiN electrode.
- Degradation of the HfO$_2$/Al$_2$O$_3$/TiN sample was not observed long time.

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DFT Study of Molecular Hydrogen Interaction with Photoexcited TiO_2 Surface: Nanocluster model

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Interaction of H_2 with photoexcited TiO_2 surface is modeled using density functional theory. Amorphous Ti_8O_{16} molecular cluster in triplet electronic state represents defect surface of the dioxide under illumination. The calculations reveal repulsion, physisorption, and dissociative photoadsorption interaction scenarios. The computed standard enthalpies of physisorption range from -0.02 to -0.11 eV. Dissociative photoadsorption proceeds on holes *via* an energy barrier (< 0.04 eV). The reaction is exothermic ($\Delta H^0 = -0.85$ eV). Neither its energetics nor the mechanism depends on the hole's stability. The calculated Ti^{3+} *g*-tensors of $Ti_8O_{16}H$ species match the experimentally observed surface Ti^{3+} EPR signal.

Fermi Level Shift Induced by Circularly Polarized Radiation in Magnetic Metal Doped BiTeI

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Recently, an interest in topological insulators and Rashba-Bychkov systems has increased due to unique properties and a high potential to be used in future generation devices they show. Some of the popular directions of spintronics investigations are a creation, a manipulation and a detection of spin currents. For example, spin current can be applied in controlled magnetic domain wall motion or used in high density memory and quantum logic architects. As it has been shown, laser with circular polarisation may create spin currents [1]. Thus, selective electron excitation from opposite branches of topological surface states in topological insulator or Rasba surface sates in Rashba systems may depend on the direction of circular polarization of applied radiation. In topological insulators opposite branches of topological surface states are spin polarized, so circularly polarized radiation may generate depopulation of Fermi level, which may be compensated by created spin current. Since the sample has a non-zero resistivity, the formation of holes at the Fermi level and spin-polarized currents should induce a redistribution of an electrochemical potential inside and outside the beam spot localization. This may be detected as an energy shift in photoelectron spectra. We suppose, that Fermi level shift can be considered as an indicator of spin currents on the surface of system.

The similar situation takes place in Rashba systems as well. Opposite branches of Rashba surface states are spin polarized as well as opposite branches of TSS, thus the similar effect of Fermi level shift may be indicated. In this work we study an existence of Fermi level shift in BiTeI and its dependence on magnetic metals doping.

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Influence of the Surface Reorganization on the Spin Electronic Structure of the Dirac Cone of Topological Insulators

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Topological insulators (TIs) represent a new quantum phase of matter, with charge excitation gaps in the bulk and gapless Dirac-cone like spin-polarized states protected by time reversal symmetry at the edge. Although the topological protection is more complete in the one-dimensional (1D) edge states of 2D TIs, such as bilayer of Bi, compared to the 2D surface states of 3D TIs, only a few works have been done experimentally because of difficulties in formation of ultrathin Bi films [1].

The intriguing phenomenon is associated with the interplay of 1D edge states and 2D surface states. A theoretical and experimental studies of single-bilayer Bi(111) ultrathin film on various 3D TIs were recently performed the presence of both types of topological states and allow to assume the occurrence of novel transport properties of such systems [2, 3].

In this work we experimentally demonstrate that the surface five-layered block of 3D TIs $Bi_2Te_{3-x}Se_x$ transforms to another compound by brief anneal of the sample. From STM, XPS and ARPES we show that new system consists of Bi Bilayer and 3D TI on basis of chalcogenides. By means of ARPES with spin and angle resolution we investigated the details of the spin and electronic structure of the formed Dirac cone, their hybridization and transport properties.

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Fabrication and Photoelectrochemical Investigation of TiO_2 Nanotubes/WO_3 Nanoparticles/TiO_2 Heterostructure

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Titanium dioxide semiconductor has received attention because of its properties, such as high photocatalytic activity in the decomposition of waste and processes arising from it: the purification of water and the formation of highly porous nanocrystalline thin films, which are useful for the preparation of, for example, dye-sensitized solar cells. The last process plays a key role in exploration of the mechanisms of photoinduced surface reactions [1]. Unfortunately, TiO_2 behavior under UV is unstable. To solve this problem we doped it with another metal.

The present work aims at the investigation of the photoelectrochemical properties of $TiO_2/WO_3/TiO_2$ heterostructure. Arrays of TiO_2 nanotubes were fabricated by anodization of Ti foils in an ethylene glycol solution containing ammonium fluoride (NH4F) under a constant voltage. In scanning electron microscope (SEM) images, we observed the microstructure of titanian nanotubes. X-ray analysis show that the as-anodized TiO_2 films come into anatase and rutile phase after the samples have been annealed at 450 °C during 7,5 h.

Followed WO_3-nanoparticals were formed on the TiO_2-substrate by liquid phase deposition method. The obtained TiO_2/WO_3 system dip-coated in the metal-organic gel based on titanium isopropoxide and annealed by 450 °C 3h. For the detection of sensitization effect in doped samples we registered the photocurrent spectra of $TiO_2/WO_3/TiO_2$-electrodes and calculated the quantum efficiency spectra η (λ), obtained I-V characteristic. Finally, we obtained the photoresponse under visible light of $TiO_2/WO_3/TiO_2$-hetrostructure.

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Electronic Structure and Chemical Bonding Features of Nickel Porphyrin NiP Studied by X-ray Absorption and Photoemission Spectroscopy

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Technological applications of transition metal porphyrins are limited due to insufficient knowledge of their electronic structure and chemical bonding. X-ray absorption and photoemission spectroscopy provides a powerful tool to obtain detailed information about occupied and unoccupied electronic states: their angular symmetry, atomic-orbital composition, energy distribution and spatial localization. The aim of the present work is to get detailed experimental knowledge of features of electronic structure and chemical bonding of nickel porphyrin NiP on the basis of comparison of its absorption and photoemission spectra with corresponding spectra of reference compounds (Ni, NiF_2, $[Ni(CN)_4]^{2-}$, H_2P) with the different type of chemical bonding.

All measurements were performed at the Russian-German beamline at the BESSY II [1] and beamline D1011 in the MAX-lab [2]. Thin films of NiP and H_2P were prepared *in situ* by thermal evaporation of porphyrin powders from a Knudsen cell and deposition of them onto Cu substrate. The metal sample was a nickel foil cleaned by scraping with a diamond file in vacuum. The samples of NiF_2 and $[Ni(CN)_4]^{2-}$ were prepared by rubbing the powder in a clean scratched copper plate. All absorption spectra were measured using total electron yield by detecting a sample current. Photoelectron spectra were collected in the angle-integrated mode using Phoibos 150 electron analyzer.

The comparative analysis of absorption, core-level and valence-band photoemission spectra of NiP allows us to state that: (i) there is a considerable role of metal-to-ligand 3dπ-2pπ* charge transfer (π-back donation); (ii) the lowest unoccupied electronic state has almost pure Ni 3d character; (iii) occupied electronic states near the Fermi level have a hybridized Ni 3d – N 2p character with a dominant contribution from Ni 3d atomic orbitals.

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Heat Capacity of Mixed Garnets at Low Temperature

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Garnets on the basis of the yttrium aluminum garnet in which yttrium ions are substituted with rare earth elements are used as laser crystals, in medicine, and other applications. An important problem of modern physics consists in understanding the low-temperature behavior of mixed garnets.

Here we present results of heat capacity studies for series of garnets with the general formula $A_{3-x}B_xAl_5O_{12}$ (where $0 \leq x \leq 3$, A - Y or Ho, B - Er, Ho, or Tm). The measurements were carried out using an automated relaxation microcalorimeter platform of the Quantum Design PPMS system in the temperature range 1.9 to 300 K. It is shown that the Yttrium substitution yields a pronounced impact on the low-temperature (< 10 K) heat capacity.

Temperature Variations of the ^{71}Ga Knight Shift in the Ternary Liquid Alloy Ga-In-Sn

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Studies of physical properties of nanostructures associated with reduction in the characteristic dimensions are in focus of modern condensed matter physics. The problem of the influence of size effects on physical properties of materials is of great practical importance in connection with the creation of new miniature devices. One way to create low-dimensional systems is the introduction of a substance into the pores of mesoporous matrices [1].

This paper presents results of NMR studies of the Ga-In-Sn alloy of the eutectic composition 77 at% Ga, 16 at% In, 7 at% Sn [2], embedded into the opal matrix. Measurements were carried out using a Bruker Avance 400 pulse NMR spectrometer at a magnetic field of 9.4 T in the temperature range from 140 to 300 K.

It was found that within the entire temperature range the ^{31}Ga resonance line consisted of two or three components. The component which was most intense at room temperature disappeared at 220 K, which corresponded to solidification of the alloy with a particular Knight shift.

The temperature dependences of the intensity of the individual components of the NMR line, which have different Knight shifts, revealed an increase in the intensity of a component at the expense of reducing the intensity of other components upon cooling the sample. This effect has not been observed till now. It is a direct proof of structural transformation in the Ga-In-Sn ternary melt under nanoconfinement.

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Unique Spin-Structure of Graphene Systems Due to Interaction with Metals

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Since A. Geim and K. Novoselov at the University of Manchester were rewarded with the Nobel Prize in Physics in 2010, the graphene became a very popular material for different kind of investigations. Such a popularity came from its extraordinary properties, for example, its high strength, chemical and mechanical stability, ability to conduct heat and electricity with very high sufficient and so on [1].

One of the most rapid developing branch among graphene researches is electronics. It is well known, that graphene features Dirac-cone like dispersion near the Fermi level in the vicinity of K point which means that graphene charge carries might be considered as massless Dirac Fermions.

Due to graphene conductive properties, it might be used as a basic material for spintronics. Spintronics is a branch of electronics which is studying the possibility of using spin-effects in it. First, we can apply graphene as a conductor of spin-current. However, the question is can we create a spin-current using graphene? The answer is yes, we can.

The main idea of this statement is to get rid of spin-degeneracy of graphene pi-states in the region of K point near the Fermi level. It is possible at least in three cases: the first one is an intensive external magnetic field, which might be obtained in graphene system using magnetic substrate. The second and the third ones are hybridization of graphene pi-states with already spin-polarized states of another material and spin-orbit interaction between electrons from graphene pi-states and cores of heavy atoms within the distance of propagation of those electrons wave functions correspondently [2].

The main goal of the current work is to show how to change graphene electronic and spin structure taking an advantage of interaction between graphene and substrate or graphene and doping atoms. Three main approaches would be presented: obtaining graphene atop magnetic structure, intercalating atoms underneath graphene monolayer and depositing atoms atop graphene.

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The Density of Unoccupied Electronic States of Ultra-Thin Phenyl Substituted Pyrrolofullerene Films

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Modification of electronic properties of organic semiconducting materials is an attractive problem due to a large potential of these materials to be a component of organic electronic devices, e.g., devices based on a single molecule. Usually ending substituents based on fullerene molecules are used for investigating of possibilities of single molecule devices thanks to the ability of covalent bonding between these ending substituents and gold atoms widely used as electrode material. The use of substituents could transform density of electronic states of organic molecules under study and change their electronic properties.

One of the ways to study of electronic properties of organic molecules is to experimentally investigate density of unoccupied electronic states (DOUS) using technics of very low energy electron diffraction provided by the total current spectroscopy method. Another one way to obtain and compare DOUS of fullerene-containing substituents is a theoretical calculation method based on the density functional theory which uses the B3LYP functional and a standard 6-31G(d) basis set.

Here we present results of comparing density of unoccupied electronic states of fullerene and aziridinphenylpyrrolofullerene (APP-C_{60}) obtained with both experimental and theoretical methods. Additionally DOUS of aziridinphenylpyrrole (APP) was calculated. The influence of attachment of APP molecule to fullerene was studied. The most pronounced changes of DOUS of APP-C_{60} relative to C_{60} observe over the range 6 to 11 eV above Fermi level. The π^* orbitals band of APP-C_{60} and C_{60} detected over the range 2 to 5,5 eV. The π^* orbitals band of APP detected over the range 4 to 6,5 eV. The mix orbitals band of APP-C_{60} and C_{60} detected over the range 5,5 to 8,7 eV. There is no mix orbitals band of APP. The σ^* orbitals band of APP-C_{60} and C_{60} begins at 8,7 eV. The σ^* orbitals band of APP molecule begins at 6,5 eV.

Effect of Preparation Method on the Valence State and Encirclement of Copper Eexchange Ions in Mordenites

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The use of zeolite in the industry has developed rapidly in recent years. Catalysis is one of the pillars of this development [1]. Copper-exchange zeolites are highly promising materials for heterogeneous catalysts and are used in numerous of chemical reactions, especially for reduction of NO*x* (de-NO*x* catalysts) [2]. Their catalytic properties are governed by both the valence state of copper ions and their location and coordination in the zeolite lattice. Moreover, the copper ion coordination is a key to fully understand reduction of copper ions incorporated into the zeolite matrix followed by the process of copper clusters formation inside zeolites. The process of hydrogen reduction of copper ion-exchange zeolites is strongly dependent on the kind of zeolite matrix, it's SiO_2/Al_2O_3 molar ratio, copper valence state and copper loading.

The method of heating (MW irradiation or conventional) during desilication of mordenite, has a clear influence on the properties of this material. Microwave irradiation of the samples promotes the Si extraction from the zeolite framework without a significant loss in crystallinity.

It is well known, that zeolite composition (SiO_2/Al_2O_3 molar ratio and counterions equilibrating the negative charge of alumosilicate framework) influence the properties of selected zeolite structure. The aim of the present study was to follow the influence of composition of the initial matrix and preparation conditions of the state of copper ions in concrete zeolite sample. We report the results of our complementary XRD,NMR, TGA and XPS study of a series of copper exchanged mordenites in different ion forms and different in SiO_2/Al_2O_3 molar ratios, obtained by two different ion-exchange methods (the conventional and MW ones).

Scientific researches were performed at Center for X-ray Diffraction Methods, Center for Chemical Analysis and Materials Research, Center for Studies in Surface Science.

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F. Optics and Spectroscopy

Brewster-Angle Reflection Spectroscopy of High-Quality GaAs/AlGaAs Single Quantum Well

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Semiconductor quantum wells (QW) is a promising object in the context of research and development of an all-optical logic element [1]. The growth technology of the most studied GaAs/AlGaAs QWs is the molecular-beam epitaxy, which allows one to produce heterostructures of very high quality demonstrating narrow spectral lines of excitonic resonances [2, 3].

In our study, sample of QW was characterized by the reflection spectroscopy in the Brewster geometry using femtosecond laser pulses as a source of probe radiation. In this case, background-free reflection spectra enabled us to analyze observed resonant lines using simple approximation of Lorentz oscillator. We approximate spectral linewidth by three main contributions: radiative linewidth, homogeneous and inhomogeneous broadenings. The radiative linewidth is proportional to the oscillator strength and oscillator density; homogeneous broadening is related to the exciton-phonon interaction, and inhomogeneous broadening is associated with the random distribution of the oscillator frequencies.

The reflection spectra were measured for the temperature range between 10 and 100 K.

It was experimentally observed that reflection coefficient decreases and spectral line demonstrates quadratic redshift and broadening with the rising temperature. It was established that radiative linewidth remains constant in this process. Extrapolation of line broadening to 0 K allows us to distinguish between temperature-dependent homogeneous and inhomogeneous broadenings.

The study was partially supported by RFBR, research project No. 14-0231617 mol-a. This work was carried out using the equipment of the SPbU Resource Center "Nanophotonics" (photon.spbu.ru).

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Dependence of ZnO Photoinduced Hydrophilic Conversion on Light Intensity and Wavelengths

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The aim of present study is to explore the effect of light intensity and spectral composition of actinic light on the efficiency of photoinduced hydrophilic conversion of the surface of ZnO nano-films. The interest in such studies connected with the wide practical application of self-cleaning surfaces, the action of which is based on the effect of photoinduced superhydrophicility. The results of this study clarify the mechanism of ZnO photoexcitation that leads to the alteration of the surface hydrophilicity.

ZnO nanofilms were received by sol-gel method.These films were analyzed by SEM and XRD. The kinetics of the contact angle on the surface of the ZnO films after the broad band irradiation was measured. The dependences of photoinduced surface hydrophilicity on light intensity and spectral distribution of photoexcitation (Fig. 1) were obtained. It is shown that hydrated ZnO surface cannot achieve the superhydrophilic state.

The analysis of the experimental data shows that photoexcitation of ZnO in both intrinsic and extrinsic absorption spectral regions leads to the formation of photocarriers and their subsequent capture of the respective surface states that, in turn, results in changing of the hydroxyl-hydrated layered structure on the surface of the water. The balance between negative and positive photoinduced surface charges dictates the surface hydrophilicity and its deviation caused by alteration of the wavelength of photoexcitation results in changing of the ZnO surface hydrophilicity.

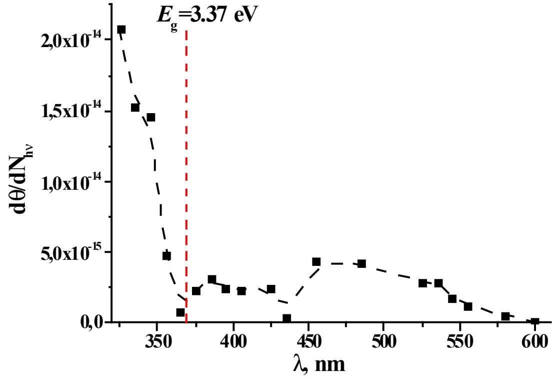

Fig. 1. The dependence of photoinduced surface hydrophilicity on spectral distribution of photoexcitation.

Analysis of Reflection Absorption Spectra of Crystal CO_2 in the Region of the ν_3 Band

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Crystal carbon dioxide is an interesting object to study, due to it is presented in several solar systems bodies and in interstellar and circumstellar ice mantles.

The IR spectra of reflection from a mirror covered with thin CO_2 crystal layers were obtained at temperature T = 77 K. The spectra in the ν_3 regions of the $^{12}CO_2$ and $^{13}CO_2$ molecules and theirs dependence on the layer thickness are discussed. The thicknesses of the layers were calculated in view of reflection from the metal surface. It was found that the shape of ν_3 band dramatically changes with increasing of layer thickness.

The ν_3 band of $^{13}CO_2$ has complex contour. The fine structure of the ν_3 band in the region of $^{13}CO_2$ absorption is explained by the resonance dipole–dipole interaction [1]. The shape of the band was calculated taking into account the interaction between two $^{13}CO_2$ molecules located in the first or second coordination sphere of each other in the regular crystal (Fig. 1).

The ν_3 band of the molecule $^{16}O^{12}C^{18}O$ was observed in this region also. This band doesn't have a complex contour, because the concentration of the 18th isotope of oxygen is low and interaction between molecules in the crystal not strong that's why the fine structure doesn't appears.

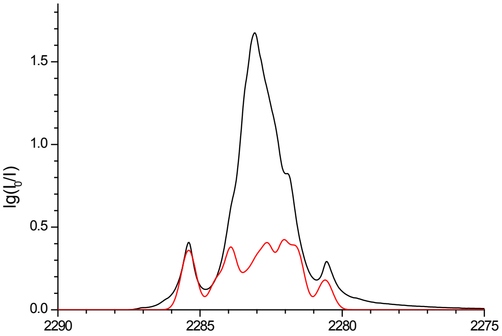

Fig. 1. The v3 band in the region of 13CO2 absorption. The black line is the experimental spectra, and the red is the calculated fine structure.

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Study of Four-Wave Mixing in Rb

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We studied the coherent multiphoton processes in the propagation of femtosecond laser pulses in optically dense rubidium vapor near atomic resonances in our laboratory. Such knowledge could be foundation for creation of all-optical switches [1] and other electronic components. These devices are needed for construction of optical and quantum computers. In recent experiments we used a femtosecond titanium-sapphire laser. Generated femtosecond laser pulse has a high intensity and wide spectral band, so we applied the excitation from the ground 5S-state to the states belonging to two different electronic configurations. First one is based on 5S-5P transition and called degenerate four-wave mixing and the second one is based on 5S-5D and 5D-6P transition and called nondegenerate four-wave mixing. Last one ends by emission of the fourth quantum with wavelength 420nm. The spatial and temporal characteristics of such processes are studied.

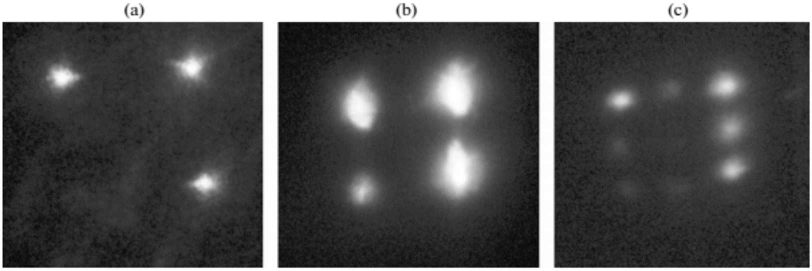

Fig. 1. Images of beams in the center plane, recorded with CCD-camera (a) no interactions (b) degenerate FWM (c) nondegenerate FWM.

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Combined Experimental and Theoretical Study of the Absorption Spectrum of the $CH_3CN…HF$ Complex

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The molecular complex of methyl cyanide (CH_3CN) with hydrogen fluoride (HF) is a very stable complex with a hydrogen bond. This complex is widely used to study the properties of hydrogen-bonded systems because of its relative simplicity. In our study the $CH_3CN…HF$ complex is studied experimentally and calculated theoretically.

The gas phase experimental spectrum was recorded in the region of the stretching vibration of HF in the complex with a resolution of 0.01 cm^{-1}. The experimental procedure and conditions were so chosen that the fine structure of spectral transitions of the complex was clearly seen.

The quantum-chemical calculation of geometrical parameters of the equilibrium nuclear configuration and the binding energy of the complex was carried out with good accuracy. Note that a full consideration of vibrations of the complex would require solution of an 18-dimensional ($3N-6 = 18$) problem that is difficult to solve. The most interesting vibrational degrees of freedom of the complex are those that appear on the H-bond formation; they are absent in free monomers. Therefore, 2D librational vibrations of the molecules, 1D H-bond and HF stretching vibrations have been considered. The results obtained in our calculation describe the most interesting vibrations of the complex provided that other vibrations are frozen. Solution of these local problems provide information about the interaction between the intramolecular and intermolecular motions. The frequencies of transitions were obtained in the harmonic (46.9 cm^{-1} (libration of CH_3CN), 177.5 cm^{-1} (H-bond stretching vibration), 681.2 cm^{-1} (libration of HF) и 3837.0 cm^{-1} (HF stretching vibration)) and anharmonic (41.3 cm^{-1} (libration of CH_3CN), 173 cm^{-1} (H-bond stretching vibration), 616.1 cm^{-1} (libration of HF) и 3586 cm^{-1} (HF stretching vibration) approximations. These calculated results are in good agreement with each other and the experimental data. This means that the method adopted in our study can be used to solve problems involving more vibrational degrees of freedom.

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Spectral-Luminescent Study of Triptycene and Energy Transfer in Triptycene Containing Systems

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The purpose of this work was a study of spectral-luminescent characteristics of triptycene, manifestations of energy transfer in doped samples and a FTIR study of sputtered films of triptycene and temperature dependence of the spectra in order to detect the crystallization of amorphous triptycene films.

The intensity of triptycene luminescence depends on the way of sample preparation and registration of the spectra. In the luminescence spectra of triptycene solutions in benzene the agregate-induced luminescence has been established.

The phenomenon of energy transfer was detected in the fused samples of triptycene modified by triazole and diphenyl, while for paradibrombenzene only superposition of the spectra of matrix and dopant was observed.

Changes in the FTIR spectra of triptycene films with temperature provide evidence for the crystallization of amorphous films on heating above 270 K.

Mixing of the $D0^+_u$ and $\delta2_u$ Ion-Pair States of Iodine Molecule

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Iodine molecule has 20 ion-pair (IP) states arranged in four tears. These states have different g/u and +/- parties and very similar potential curves. These features make the IP states very convenient for observation of the heterogeneous perturbations and hyperfine interactions. Previous studies [1, 2] have indicated that both of these mechanisms are observed in IP states of iodine molecule.

The study has shown that optical population of the iodine molecule $\delta2_u$ state is observed due to nonadiabatic interaction of this state with the $D0^+_u$ one (Fig. 1). So, the luminescence from the $\delta2_u$ state become discernible because of mixing of $D0^+_u$ and $\delta2_u$ IP states for the first time. Results have proved the mechanism of the heterogeneous interaction between above-mentioned rovibronic levels in the second order of the perturbation theory. Earlier, similar NO ($B^2\Pi/C^2\Pi/D^2\Sigma^+$) 'indirect' heterogeneous interaction was observed in [3].

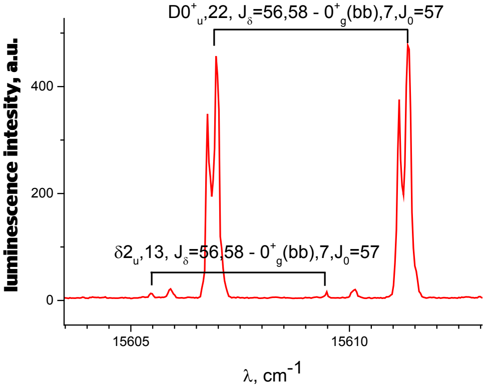

Fig. 1. Excitation spectra of the luminescence corresponding to the D,22,J_D=56,58 → X and δ,13, J_δ=56,58 → 2_g(aa) transitions.

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On Mutual Consistency Between Wavelength and Wavenumber Values for Electronic-Vibro-Rotational Lines of the H_2 Molecule Reported in Tables of G.H. Dieke

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Electronic-vibro-rotational spectrum of the H_2 molecule is extensively used in quantitative spectroscopy of ionized gases and plasmas. Currently the Tables of G.H.Dieke [1] is the most complete data compilation about emission spectrum of H_2. They contain wavenumbers of spectral lines ν_i, wavelengths in air λ_i^{air} and vacuum λ_i^{vac}; eye estimates of the line intensities for various experimental conditions; references to earlier works; as well as assignments for some lines in the wide spectral range from near ultraviolet up to far infrared. In the most important for various applications visible part of the spectrum (4000-7000 Å) the tables contain the data about 17882 spectral lines. These data were not verified by any statistical analysis, in contrast to that made for the D_2 molecule [2]. The goal of the present work was to study a mutual correspondence between ν_i, λ_i^{air}, and λ_i^{vac} for visible part of the spectrum. Our calculations show that for the vast majority of spectral lines there is significant inconsistency between values λ_i^{vac} and $1/\nu_i$. Then, the pairs of values λ_i^{air} - λ_i^{vac} were used for calculating the dependence $n(\lambda_i^{air})$ of the air refraction index used by G.H. Dieke. The sawtooth structure of this dependence was found. Certain analysis made it possible to find out that both effects (the sawtooth structure of $n(\lambda_i^{air})$, and the λ_i^{vac} - $1/\nu_i$ inconsistency) have common origin. The λ_i^{vac} values reported in [1] were obtained from experimental values λ_i^{air} by adding certain corrections $\Delta\lambda_i$ (accounting the $n(\lambda_i^{air})$ dependence) with the fixed step value 0,001 Å. The approximation of $n(\lambda_i^{air})$ by proper analytical function made it possible to reveal and correct various misprints, and to obtain new values for λ_i^{vac} and $\nu_i=1/\lambda_i^{vac}$. Thus, new self-consistent set of values (λ_i^{air}, λ_i^{vac}, ν_i) is obtained for spectral lines of the H_2 molecule located in the wavelength range 4000-7000 Å.

This work was supported in part by the RFBR foundation (project No. 13-03-00786a).

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Specific Features of Short-Range Order in Mesogenic Compound Melts

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Electro-optical studies of isotropic mesogenic polymer melts showed that some high-molecular compounds could have two isotropic phases with different properties and a transition between them. This transition is observed either in the copolymer [1], or in a chiral smectic polymer [2, 3]. Calorimetry methods [4-6] and dielectric spectroscopy [7] previously established the existence of such transitions in isotropic melts of low molecular chiral mesogens.

Isotropic - isotropic phase transitions were also found in melts of non-chiral smectic comb-like polymers with mesogenic side groups [8]. Thus, it has been shown that these transitions appear in smectic polymers with different structure of the main chain and side groups. In this regard, the question about the causes and nature of transitions in the isotropic phase of the polymers and the role of the side mesogenic groups in such transitions arises.

In this paper, we investigated the electro-optical properties of nematic 4-n-pentyl-4'-cyanobiphenyl. For this, several series of high precise measurements in a wide temperature range were carried out, and the existence of a structural transition in the isotropic phase was established. In this case the change of the dependence of inverse Kerr constant 1/K with temperature T indicates the presence of structural transition for this sample.

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Stratification of Discharge in Noble Gases from the Viewpoint of the Discrete Dynmaics

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Gas-discharge plasma stratification is one of the fundamental problems of non-equilibrium plasma physics. In recent years, considerable progress was reached by a better understanding of the generation and propagation mechanisms of stratification under different discharge conditions. Currently, two main approaches are generally used to describe striations, a fluid and a kinetic one.

A new point of view on the nature of stratification of discharge in noble gases based on the analysis of phase trajectories of electrons in the "kinetic energy - coordinate" phase plane was considered [1]. The problem of striation generation in a positive discharge column was interpreted as the formation of integer and non-integer resonances due to the specificity of the nonlocal behavior of electrons in noble gases at lower currents.

The goal of the present work is to develop the dynamics theory of stratification. For this purpose elastic collisions interference was analyzed.

Due to this model main properties of resonant trajectories (Fig. 1) and the variety of possible striation types in the positive column can be predicted by solving one simple differential equation (Fig. 2).

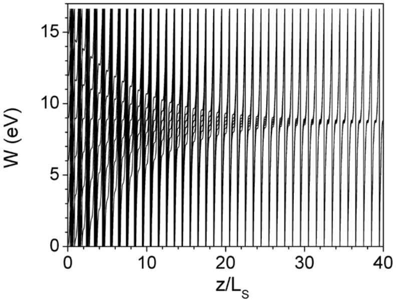

Fig. 1. Phase trajectories convergence to the resonant one.

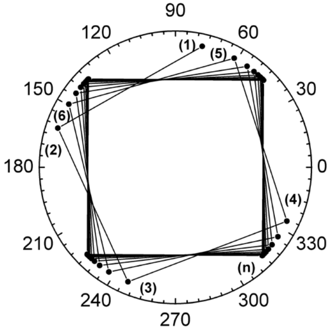

Fig. 2. Solution of the equation describing convergence to the attractor.

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Analysis of Time-Resolved Luminescence Spectra of Ion-Pair States of Iodine Molecule

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At the present time, iodine molecule stillattracts attention of researchersall over the world thoughit has been already studied quite well. Iodine is widely used both in fundamental and applied sciences. It can be used as a model system for investigations of molecular processes in gaseous phase. Moreover, it can be used as active media in chemical lasers.

Time-resolved spectroscopy is a widely used tool in the photophysics, photochemistry and photobiology for studies of the dynamic properties of complex systems [1]. In the present work, analysis of time-resolved luminescence spectra of first tier ion-pair states of iodine molecule was provided (Fig. 1). The result of analysis arepartial luminescence spectra as well as partial rates constants of collision-induced non-adiabatic transitions between ion-pair states.

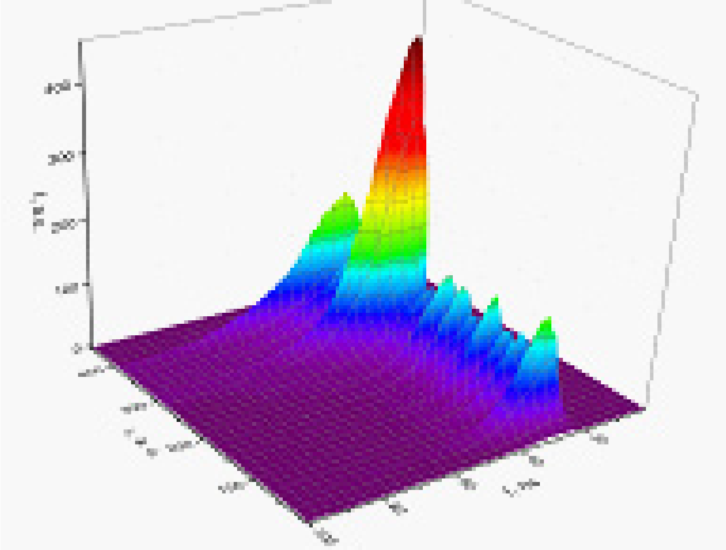

Fig. 1. Time-resolved luminescence spectra of ion-pair states of iodine molecule.

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Near-resonant Raman Scattering From Valence State via Iion-Pair States in Iodine Molecule

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Raman spectroscopy is well known and widespread method to investigate molecular structure. There are about 25 types of Raman spectroscopies used by modern researchers [1]. Nevertheless some aspects remain unexplored experimentally until now. This is the case for electronic and vibronic Raman scattering from highly excited states. As for diatomic molecules, the theory of these effects was developed in 1970's [2], but nobody observed it.

This work is devoted near-resonant Raman scattering from 0_g^+ (*bb*) valence state via ion-pair states in iodine molecule. The feature of the study is three-step three-color laser excitation scheme:

$$I_2(D0_u^+,22,51 \xleftarrow{h\nu_2} 0_g^+(bb), 7, 52 \xleftarrow{h\nu_f} B0_u^+,21,53 \xleftarrow{h\nu_1} X0_g^+,0, 52)$$

In the last step of excitation we observe both population of the $D0_u^+$ state and perturbation of the molecule, which produces scattering radiation. Measured scattering spectrum lies in far anti-Stokes region. Using the time-resolved spectroscopy allows us to separate weak Raman scattering from intense luminescence background.

As a result, we concluded, that luminescence and Raman scattering spectra are identical. The spectral dependence of the scattering intensity was studied and compared with results of theoretical predictions, also. Finally, we found the presence of near-resonant Raman scattering via another ion-pair states of iodine molecule.

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G. Theoretical, Mathematical and Computational Physics

Nuclear Recoil and Vacuum-Polarization Effects on the Binding Energies of Supercritical H-like Ions

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The well-known Sommerfeld formula for the case of a point nucleus describes the electronic spectrum of hydrogenlike ions only for $Z < 137$ (Z is the nuclear charge). When Z becomes greater than 137, one can employ the model of an extended nucleus [1-3] which provides an adequate solutions for all values of Z. In Ref. [4] a supercritical H-like ion was analyzed by decreasing the nuclear radius and it was shown that the interaction with a point charge in quantum electrodynamics (QED) cannot effectively have the coupling strength of 1 or greater (the corresponding effective charge is 137).

In present work this statement is revised in the presence of the recoil and vacuum polarization operators. It turned out that these effects significantly change the pattern described previously. It was found that the nuclear recoil operator within the Breit approximation "regularizes" the Dirac Hamiltonian for the point-nucleus model and allows the nucleus to have an arbitrarily large charge. This means that the effective charge of a point-like particle can be greater than 137 once its mass is finite.

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Spectrum of the Generalized Tavis-Cummings Model

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Strong light-matter interaction is one of the central subjects in quantum information processing. The exactly solvable models of quantum nonlinear optics provides a natural platform for studies in this direction. Very recently these models have again attracted attention. The model which describes N two-level atoms interacting with a single mode of a cavity field, solved exactly by solved exactly by Tavis and Cummings [1].

If the cavity is not ideal because the cavity mode is coupled to a Kerr-like medium, an effective Hamiltonian can be derived which adds a fourth-order term in the boson operators to the simple JC Hamiltonian. The Tavis-Cummings (TC) model with the Kerr nonlinearity belongs to a different set of integrable models. It was solved by the Quantum Inverse Method (QIM) in [2]. To obtain the detailed information about the behavior of the intrinsically nonlinear models the exact expressions for the dynamical correlation functions is necessary to know. In this work we have derived the spectrum of the generalized TC model by QIM, what is necessary for further calculations of correlation functions.

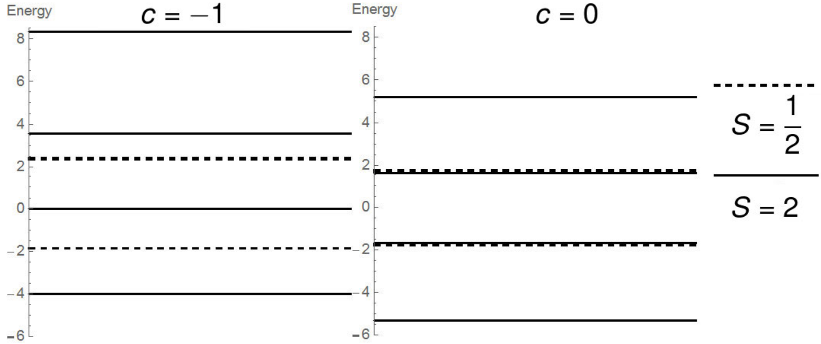

Fig. 1. Comparison of TC model M-particle eigenenergies (M=3) in presence of Kerr nonlinearity c=-1, and absence c=0, for zero detuning.

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Ultrafast photochemistry of $CuCl_4^{2-}$ complex in acetonitrile by means of transient absorption spectroscopy and TD-DFT calculations

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In this work, we reported detailed description of the ultrafast dynamics of a $CuCl_4^{2-}$ complex in acetonitrile upon excitation into all possible Ligand Field (LF) states due to transitions between d-orbitals of the Cu^{2+} ion, and three most intense Ligand-to-Metal Charge Transfer (LMCT) transitions. The LF states are found to be nonreactive states, while excitation into the LMCT states leads to the ionic dissociation of $CuCl_4^{2-}$ complex followed by the recombination into parent complex.

The mechanisms of the relaxation of the LF and LMCT excited states were proposed form the femtosecond transient absorption laser spectroscopy measurements. The lifetimes of three possible LF excited states were determined. Thus lowest lying ^2E LF excited state has the lifetime about 50 fs, intermediate $^2B_1$ LF excited state is characterized by the lifetime equal to 1 ps, and highest-energy LF state of the $CuCl_4^{2-}$complex, $^2A_1$, has a lifetime about 5 ps. Such humongous difference in lifetimes was explained from theoretical point of view by Time-Dependent Density Functional Theory (TD-DFT) calculations. The conical intersection between $^2B_2$ ground state and ^2E LF excited state was discovered, whereas $^2B_1$ and $^2A_1$ LF excited states do not cross either ground electronic state or each other. The Franck-Condon mode is found to be symmetric Cl-Cu-Cl bending vibration.

Majority of the short-lived LMCT excited states undergo internal conversion to the lower-lying vibrationally hot LF excited states, which then either nonradiatively decay to the ground state, whereas minor number of LMCT-excited complexes undergo Cu-Cl ionic bond dissociation, forming $CuCl_3^-$ and Cl^- ions, which then recombine re-forming parent complex. In case of LMCT excitation the Franck-Condon mode is ought to be asymmetric Cl-Cu stretching vibration.

Acknowledgments

Calculations have been made with the assistance of the Saint-Petersburg State University Computer Center. This work was supported by the NSF CAREER award (Grant CHE-0847707), NSF MRI program (Grant CHE-0923360), Saint Petersburg State University research grants (2015–2017, 12.38.219.2015), and RFBR (Grants 14-03-01003 and 15-03-05139).

Computation of Water Drops Electrocoalescence in a Dielectric Liquid

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Electrocoalescence is a process of droplets unification under the effect of the electric field [1]. This phenomenon is of great interest since it underlies the technology of crude oil purification as well as can be used for micro drops mixing in pharmacy.

The paper deals with problems concerning the application of standard two-phase-media model to the description of water drop deformations under the effect of the electric field. The available computer models lead to the emergence of space charge far from the droplet boundary (the so-called charge runaway problem).

The computations were performed in 2D and 2D axial statements using software package COMSOL Multiphysics. The comparison of the results obtained in classical and new model are presented. The application of the new model (Fig. 1) increases the correctness of the physics description of two-phase-media motion under the effect of the electric field.

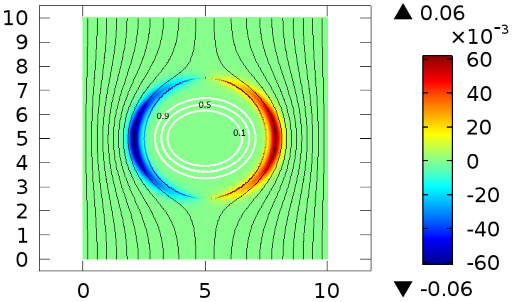

Fig. 1. Surface plot of Volume charge.

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How Super Yang-Mills Theories Can Help Us to Understand Confinement

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It is well known fact that strong interactions enjoy a confinement phenomenon. This follows from the real-world experiments and from numerical calculations, but so far no one succeeded to derive this property from the modern theory of strong interaction with gauge group SU(3). It is believed that the effect is essentially non-perturbative.

In the case of supersymmetric theories, however, some data can be computed in strong coupling even if the full theory cannot be solved. This happens when theory has BPS sector. Example of such theory is the SU(N)×U(1) N = 2 QCD, and studying it provides deep insights in non-supersymmetric quantum chromodynamics and other non-supersymmetric theories.

Physical scenarios in different vacua of N=2 supersymmetric QCD deformed by the mass term μ for the adjoint matter are considered. Due to this deformation theory goes to N=1 QCD. Monopole-antimonopole pairs are confined by non-Abelian strings.

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Multi-Loop Calculation of Critical Exponents in the Model E of Critical Dynamics

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In this paper we consider a dynamic model E, which describes a symmetric planar antiferromagnetic.

Physical interest is to find the dynamical critical exponent z, which determines the growth of the relaxation time near the critical point in the (d = 4 – 2 epsilon) epsilon-expantion framework for the model E of critical dynamics.

The result, which was previously made, do not give us an answer, so it is necessary to make calculation of higher-order perturbation theory. The main outcome of this work is obtaining of two loop results for RG functions determining the critical model exponents.

Relativistic Calculations of Excitation and Ionization Probabilities in H-like Ions Exposed to an Intense Laser Field

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Nowadays, laser technologies are rapidly developed and highly charged ions are ones of the most interesting objects that can be studied with intense laser fields [1, 2]. The time-dependent problems including an interaction with intense laser fields attract much attention during the past few years [3, 4].

In this work, a new method and code were designed for the investigation of highly charged ions exposed to an intense laser field. The theoretical consideration of this problem requires to solve the time-dependent Dirac equation. The method for solving the Dirac equation is proposed within the dipole approximation of a laser potential.

Based on the method developed, excitation and ionization probabilities were calculated for various ions [5]. For instance, the multiphoton ionization process for the hydrogenlike tin ion ($Z = 50$) was investigated. The laser potential was chosen in the form of linearly polarized 20-cycle $\cos^2$-shaped pulse with a peak intensity of $5 \cdot 10^{22}$ W/cm^2. The ionization probability was calculated in both length and velocity gauges. The results obtained in two gauges coincide with each other. Moreover, our results are in good agreement with the corresponding data from Refs. [3, 4].

Also, the method developed was applied to calculate transition probabilities. The electric field is chosen in the form of Gaussian-shaped laser pulse with a peak intensity of $6.8 \cdot 10^{19}$ W/cm^2. As an example, the transition probabilities from the initial 1*s* state to the excited states in the H-like argon ion ($Z = 18$) due to the interaction with a laser pulse were calculated.

The investigations made are expected to be required for the future High-Intensity Laser Ion-Trap Experiment (HILITE) [2].

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Effects of Random Environment on a Self-Organized Critical System: Renormalization Group Analysis of a Continuous Model

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We study effects of random fluid motion on a system in a self-organized critical state. The latter is described by the continuous stochastic model, proposed in [1]. The advecting velocity field is Gaussian, not correlated in time, with the pair correlation function of the form

$$\sim \delta\left(t-t'\right)/\,k_{\perp}^{d-1+\xi}$$

where $k_{\perp} = \left|k_{\perp}\right|$ and $k_{\perp}$ is the component of the wave vector, perpendicular to a certain preferred direction – the d-dimensional generalization of the ensemble introduced in [2]. Using the field theoretic renormalization group we show that, depending on the relation between the exponent ξ and the spatial dimension d, the system reveals different types of large-scale, long-time scaling behaviour, associated with the three possible fixed points of the renormalization group equations. They correspond to ordinary diffusion, to passively advected scalar field (the nonlinearity of the Hwa– Kardar model is irrelevant) and to the "pure" Hwa–Kardar model (the advection is irrelevant). For the special choice ξ=2(4-d)/3 both the nonlinearity and the advection are important. The corresponding critical exponents are found exactly for all these cases.

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Computer Simulation Study of Bragg Peak in Simple Heterogeneous Model of Biological Object

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Cancer treatment is one of the most meaningful branch of the medicine in our days. Almost half of all people with cancer have radiotherapy as part of their treatment plan. The main criterion used in all radiotherapy techniques is to deliver a sufficient dose to achieve tumor while minimizing side effects. In this case use of light nuclei, e.g. carbon ions, have an additional advantage compared to protons associated with their enhanced relative biological effectiveness [1].

Computational physics allows us predict the biological response with accuracy necessary for therapy planning. So in this work was used a Geant4 toolkit [2] to simulate the passage of carbon through homo- and heterogeneous matter and calculate depth-dose distribution (Fig. 1).

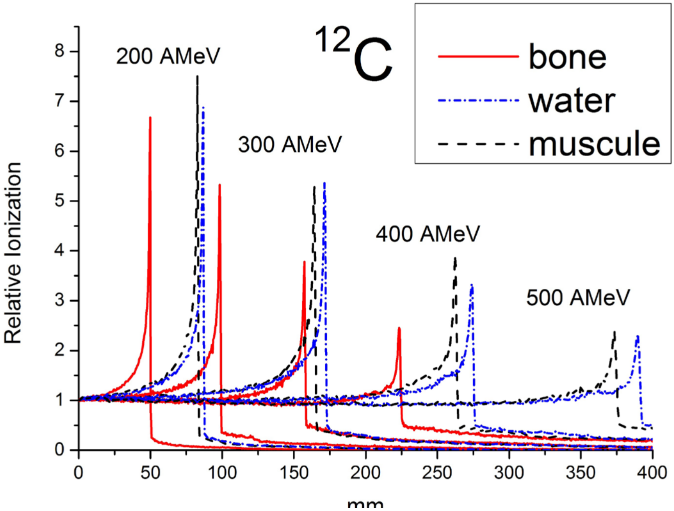

Fig. 1. Carbon Bragg peak curves for different materials.

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Holographic Study of the QCD Matter Under External Conditions

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The bottom-up approach to the holographic AdS/QCD (anti-de Sitter/Quantum Chromodynamics) correspondence is considered. It is based on the hypothesis of AdS/CFT (anti-de Sitter/Conformal Field Theory) duality and represents a new tool to investigate the strongly interacting regime of gauge theories. Confinement, chiral symmetry breaking and the structure of the QCD phase diagram represent a range of problems into which the AdS/QCD correspondence gives a new insight.

One of the primary questions in Quantum Chromodynamics is the clarification of the whole phase diagram of matter out of quarks and gluons as a function of temperature, baryon or quark chemical potential, and other external parameters. This knowledge is of a great pragmatic interest as it is essential for the understanding of laboratory experiments involving relativistic heavy-ion collisions such as carried out at LHC, RHIC and in future at FAIR.

We focus on determination of conditions of transition from the confining to the deconfining phase of quark matter. In AdS/CFT and AdS/QCD models such transitions are supposed to be the Hawking-Page transitions between spacetimes with different geometries. It is believed that in QCD deconfinement occurs as a rapid crossover, not a phase transition. While the Hawking-Page transition is a first-order phase transition, one can find values of critical parameters (like the deconfinement temperature).

Starting with a particular bottom-up AdS/QCD model we find quantitative expressions for such critical parameters. The way input phenomenological and theoretical model parameters affect predictions of the value of the critical temperature and chemical potential is studied in detail. Comparison of model predictions with results of experimental investigations, lattice QCD simulations and other methods is done.

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Renormalization Group Approach to Turbulence

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The field theoretic renormalization group and the operator product expansion are applied to the model of passive vector (magnetic) field advected by a random turbulent velocity field. The latter is governed by the Navier–Stokes equation for compressible fluid, subject to external random force with the covariance

$$\propto \delta(t-t')k^{4-d-y},$$

where d is the dimension of space and y is an arbitrary exponent. From physics viewpoints, the model describes magnetohydrodynamic turbulence in the so-called kinematic approximation, where the effects of the magnetic field on the dynamics of the fluid are neglected. The original stochastic problem is reformulated as a multiplicatively renormalizable field theoretic model; the corresponding renormalization group equations possess an infrared attractive fixed point. It is shown that various correlation functions of the magnetic field and its powers demonstrate anomalous scaling behavior in the inertial-convective range already for small values of y. The corresponding anomalous exponents, identified with scaling (critical) dimensions of certain composite fields ("operators" in the quantum-field terminology), can be systematically calculated as series in y. The practical calculation is performed in the leading one-loop approximation, including exponents in anisotropic contributions.

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Solutions of the Nonstationary Schrödinger Equation in an External Constant Uniform Magnetic Field

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Solutions of non-stationary Schrödinger equations [1] play an important role in many tasks of Theoretical Physics. Because many processes that we can observe in experiments should be described in non-stationary case, we want to see the evolution of these processes. In the simplest case, we can describe a free particle; the solution in this instance takes a form as follows:

$$|\Psi|^2 = \frac{P_0}{\hbar\sqrt{\pi\left(1+\frac{P_0^4 t^2}{m^2\hbar^2}\right)}} Exp\left\{-\frac{\left(\frac{P_0}{\hbar}(x-v_0 t)\right)^2}{\left(1+\frac{P_0^4 t^2}{m^2\hbar^2}\right)}\right\}$$

If the particle is a fermionis in rotating magnetic field, then it's spin dynamics can be described with the following density of the probability function:

$$P(t) = \langle\Psi_2|\Psi_2\rangle = \frac{\Omega^2}{\tilde{\Omega}^2}\sin^2\frac{\tilde{\Omega}t}{2} = \frac{\Omega^2}{\Omega^2+(\omega-\omega_L)^2}\sin^2\frac{\tilde{\Omega}t}{2}$$

Dynamics of the charged particle in constant magnetic field can be described in the same terms, but density of the probability function cannot be shown here because its expression is cumbersome. If we apply the correspondence principle to this task, we'll get the following result:

$$\lim_{\hbar\to 0}|\Psi|^2 = \delta(x-x_0+R\cos(\omega t+\varphi))\delta(y-y_0+R\sin(\omega t+\tilde{\varphi}))\delta(z)$$

Given the delta function arguments be zero, we obtain the classical trajectory of a charged particle in a constant magnetic field.

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One-loop Divergences for the Effective Action in the Weinberg-Salam Model

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It is known that quantum corrections to the classical Yang-Mills action (see for example[1]),

$$\frac{1}{4g^2}\int B^a_{\mu\nu}B^a_{\mu\nu}\,dx$$

in the one-loop approach give

$$\frac{1}{4}\left(\frac{1}{g^2}+\frac{11}{48\pi^2}C(G)\ln\frac{\epsilon}{\mu}\right)\int B^a_{\mu\nu}B^a_{\mu\nu}\,dx+$$

$$+\ \text{finite zero order terms}\ +\ \text{higher order loops}$$

After that you can do the renormalization in the spirit of the Landau-Wilson :

$$\frac{1}{g^2(\epsilon)}+\beta\ln\frac{\epsilon}{\mu}=\frac{1}{g^2_{ren}}$$

In this paper the one-loop corrections are calculated in the formalism of the external field for the modified Lagrangian to the Weinberg-Salam model, which does not include the mass term and the Higgs potential. It is shown that these terms appear in the action, so a proposal discussed in the article [2], required further discussion. Also in the paper first coefficient of the Gell-Mann-Low (**β**-functions) for the gauge fields were calculated, and the signs for the Abelian and non-Abelian fields differ. The main result of this note is the fact that the one-loop corrections to the classical Lagrangian

$$\mathscr{L}_0=(\nabla_\mu\Psi,\nabla_\mu\Psi)+\frac{1}{4g^2}B^a_{\mu\nu}B^a_{\mu\nu}+\frac{1}{4g'^2}Z^2_{\mu\nu}$$

lead to the Lagrangian of the form

$$\mathscr{L}_0\ \to\ \mathscr{L}=\left[1+\beta_1\ln\frac{\varepsilon}{\mu}\right](\nabla_\mu\Psi,\nabla_\mu\Psi)+\left[\frac{1}{4g^2}+\beta_2\ln\frac{\varepsilon}{\mu}\right]B^a_{\mu\nu}B^a_{\mu\nu}+$$

$$+\left[\frac{1}{4g'^2}-\beta_3\ln\frac{\varepsilon}{\mu}\right]Z^2_{\mu\nu}+\ln\frac{\varepsilon}{\mu}\left(\beta_4|\Psi|^4-\beta_5\partial^2|\Psi|^2\right)-\beta_6\left(\frac{1}{\varepsilon^2}-\frac{1}{\mu^2}\right)|\Psi|^2,$$

where β_k are the positive constants depending on coupling constants.

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Non-leading Light-Cone Distribution Amplitude of B-Meson

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B-meson is also known as the open-beauty heavy meson which consists of the light *u*- or *d*-quark and heavy *b*-antiquark. In the Heavy Quark Effective Theory (HQET) framework, the heavy antiquark is considered as the stationary source and the meson dynamics is completely determined by the motion of the light quark. From the phenomenological point of view, decays of *B*-mesons are described by transition matrix elements from the *B*-meson state into the vacuum or hadronic one. If we restrict ourselves the transition matrix element from the *B*-meson state to the vacuum, there are two functions only which are called leading and non-leading Light-Cone Distribution Amplitudes (LCDAs). There are three models for the leading LCDA [1-3] which are widely used in applications. Lee and Neubert [4] suggested the modified form of the model [1] which is matched with the asymptotic form following from the perturbative QCD. The non-leading LCDA can be related with the leading one by virtue of the Wandzura-Wilczek relation [1]. Both leading and non-leading LCDAs are calculated within the simplest models [1, 2] but two other, more complicated models are presented by the leading LCDA only. We have calculated the non-leading LCDA related with the models [3, 4] in the Wandzura-Wilczek approximation. Using these LCDAs the momentum-transverse-dependent first inverse moments have been calculated which are of impotence, for example, in the analysis of exclusive radiative, semileptonic and hadronic decays of *B*-mesons.

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Critical Behavior of the Systems with a Real Tensor Order Parameter: Three-loop Approximation

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Numerous physical systems reveal interesting singular behavior in the vicinity of their critical points. Their thermodynamical and correlation functions exhibit scaling behavior with universal critical dimensions: according to general belief, they depend only on a few global characteristics of the system, such as symmetry or dimension. The powerful and quantitative theory of the critical behavior is provided by the field theoretic renormalization group (RG). In the RG approach, possible types of critical behavior are associated with infrared attractive fixed points of renormalizable field theoretic models.

In the present work the field theoretic renormalization group is applied to the O(n)-symmetric phy4 model of the real n-th rank tensor order parameter [1]. This model can be relevant in the analysis of transitions between the nematic, cholesteric and blue phases in liquid crystals, transitions to the ferroelastic state in solids and transitions to the superconductive state in systems with higher spins. RG-functions of the model were calculated in three-loop approximation. The critical exponents were presented in the form of series expansion by the deviation of the spatial dimension from its logarithmic value in the same approximation. In order to obtain the numerical values of the critical exponents at physical value of spatial dimension the asymptotic of high orders of perturbation theory was studied [2]. Final results were obtained by resummation of previously calculated segments of the series expansions by method of conformal transformation of Borel [3].

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Classical Gravitational Effects of Massless Cosmic Strings

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For the first time we investigated a series of gravitational effects of massless cosmic strings. A massless cosmic string is a linear object which is moving at the speed of light [3, 4, 6, 7]. It is shown that massless cosmic strings can lead not only to mutual space rotations of reference systems related to the observers, whose trajectories are on different sides from the string, but also to a further mutual motion of observers. As a result of this effect the light rays in the gravitational field of the string could change not only the direction but also the frequency according to the Doppler Effect. These results are right for a single string and for a continuous sequence of strings which have a finite energy distribution in the direction of motion.

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Computer Simulation of Flight Facility Based on Ionic Wind

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When high voltage is applied between two electrodes, electrons accelerate in electric field and gain energy large enough to ionize air molecules. So avalanche increasing number of charged particles – positive (ions) and negative (electrons) ones – takes place. Discharge called corona discharge is formed in inhomogeneous electric fields. The charged particles acquire the momentum from electric field and quickly transfer it to air molecules at collisions. As a result the air comes in regular motion as a whole. Electrohydrodynamic flow originates – called ionic wind. The reactive jet force of ionic wind can be used as a lifting force.

The numerical calculation of lifting force of flight facility – ionocraft (Fig. 1) – is performed using the Comsol Multiphysics software package based on the finite element method.

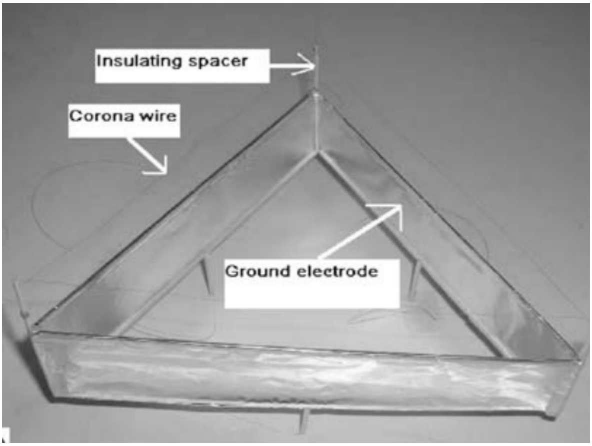

Fig. 1. Picture of the flight facility.

Profiled Conductive Coating on a Solid Dielectric Insulation

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The conductive coating on the solid insulator is used to smooth the electric field in high-voltage insulation. High-voltage devices should be tested under the influence of the short voltage pulses (“standard lightning pulse”; tens of microseconds) and power frequency voltage. Using a coating with a uniform conductivity becomes difficult in this situation. The coating conductivity value should be sufficient to smooth potential within microseconds (short voltage pulses). Applying this conductivity by power frequency voltage results in strong electric currents which may damage insulation. A possible way to solve this problem is to use a coating composed of alternating bands of high and low conductivity. Computer simulation is performed to verify this method. The achieved insulation characteristics are sufficiently better than ones of the uniform coating. However the field intensity in the solid insulation is sufficiently high in a small area. The question of the admissibility of such areas requires further study.

Application of Scattering Theory for Computation of the Casimir Forces Between Two Periodic Media

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Casimir effect is a macroscopic quantum effect based on vacuum fluctuations. It was predicted by H. B. G. Casimir in 1948 who considered two parallel perfectly conducted plates separated by a vacuum slit and derived the result for the attractive force between the plates [1]. Later the effect was supported by many experiments and nowadays great attention is paying on it.

The theoretical formalism for the case of two media periodic in one spatial direction and translationally invariant in the orthogonal direction was developed in Ref. [2].

In the present work we study Casimir effect for two media periodic in two orthogonal directions separated by vacuum (Fig. 1), frequency dependence of the media dielectric permittivities is assumed. We use Rayleigh decompositions [3] to evaluate the Casimir free energy. Our work is based on the scattering theory for the case of two media periodic in orthogonal directions.

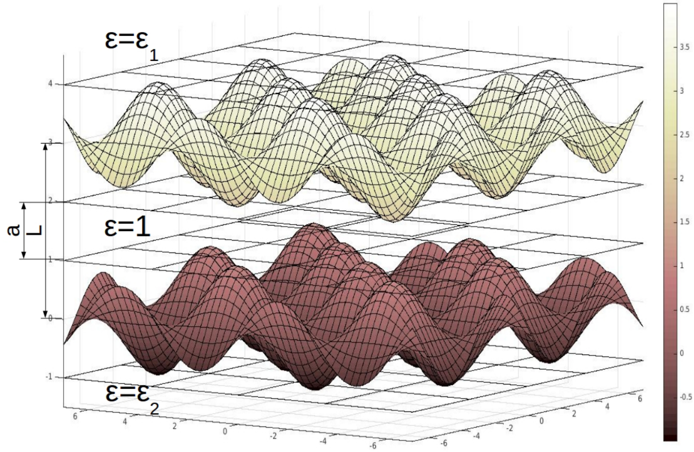

Fig. 1. Two media periodic in two orthogonal directions.

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Relativistic Calculations of Transition Probabilities in Hydrogen-like Ions

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Accurate values of transition probabilities in hydrogen-like ions are needed for many practical applications in various realms of physics. For example, they are demanded for interpretation of the spectra from astrophysical sources and in researches of characteristic photon emission in recombination and other scattering processes. To date, the systematic theoretical data for the transition probabilities in hydrogen-like ions are mainly restricted to the point-charge nuclei [1, 2] while most of the current calculations are carried out for extended-charge nuclei.

In the present work, the transition probabilities in hydrogen-like ions with nuclear charges in range $Z=1-100$ were evaluated taking into account the effect of finite nuclear size. The calculations were carried out by two different methods and in two gauges: length and velocity. The calculations of the Dirac wave functions were performed using the RADIAL package [3]. All the results obtained by two different methods coincide with each other.

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Simulation of Heat Transfer Enhancement by Virtue of the Electric Field

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The electrohydrodynamic (EHD) flow is a special type of flow that emerges under the effect of the electric field. The flow can be used for cooling different areas in a small scale, e.g. to cool computer chips. The corresponding devices are called EHD heat exchangers.

The available models of EHD heat exchangers are simplified ones since they disregard electric conductivity. The present paper considers a more complete model that allows one to compute characteristics of the EHD heat exchanger.

The blade-plane electrode system and two models of charge formation (the injection and dissociation) are considered in the simulation. The dependence of heat flux from the electric conductivity was obtained (Fig. 1).

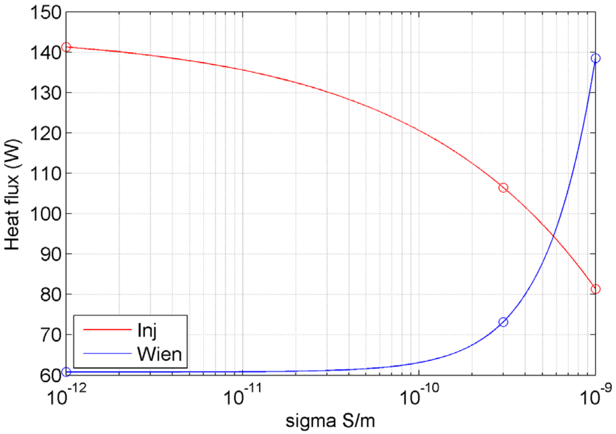

Fig. 1. The dependence of heat flux from the electric conductivity.

Gluonic Light-Cone Distribution Amplitudes of Pseudoscalar Flavor-Singlet Meson

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Light scalar and pseudoscalar mesons are of special interest in particle physics since the foundation of the strong interaction theory called Quantum Chromodynamics (QCD). The non-abelian nature of the theory allows to explain the existence of hadrons (mesons and baryons) based on the confinement of quarks but, in addition, suggests a new type of mesons called glueballs [1] which are pure states constructed from gluons only. There is no an experimental evidence of glueballs at present. Nevertheless, the mixing of states with the same quantum numbers J^P (the spin J and parity P) allows to observe the pure gluonic states as the admixture to the usual mesons. In particular, the two-gluon component with the quantum numbers $J^P=0^-$ can mix with the neutral flavor-singlet pseudoscalar meson. With an account of the existing mixing of the $SU_F(3)$-octet states and flavor-singlet one, the two-gluonic state can be found as a component in the η- and η’-meson wave-functions and decay modes induced by this component have been observed experimentally [2].

The method of constructing the quark-antiquark pseudoscalar interpolation currents for light pseudoscalar mesons is learned in details on the π^+-meson wave-function as an example. When the π^+-meson is a fast-moving particle its wave-function is considerably simplified and can be written in terms of Light-Cone Distribution Amplitudes (LCDAs) of increasing twist. In the η- and η’-mesons the set of interpolating currents should be extended by introducing the gluonic interpolating currents which results to additional LCDAs. An attempt to study some of these LCDAs was recently undertaken in Ref. [3] but more detail analysis of gluonic LCDAs of pseudoscalar mesons is still necessary. The interpolation currents of the twist-3 (skipped in [3]) was considered by us and the corresponding asymptotic forms of LCDAs are presented based on the conformal symmetry. The mixing of these states with the conventional (quark-antiquark) ones as the result of the current renormalization is planning to be worked out.

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Determination of the Polar Angles of Recoil Particles Measured with the Active Target Detector (ACTAR) of the R3B Setup with ROOT-based Programs

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The R3B setup is aimed for the complete measurements of reactions with heavy ion beams including detection and identification of heavy residues, as well as neutrons, protons and photons. Different kinds of its detector systems allow to run the experiments with different types of reactions and physical cases.

Active target detector (ACTAR) is supposed to be a part of the R3B setup. It will allow registration of the recoil particles in coincidence with the heavy fragments, neutrons and gamma-rays. This setup gives thus a unique possibility to study elastic, inelastic, knockout and breakup reactions at low momentum transfer, and it will extend the possibilities of R3B in studies of nuclear structure of light and heavy exotic short-lived nuclei [1,2].

The main aim of this work was determination of the polar angle of recoiled particles with ROOT-based programs (Fig.1). ROOT-based specially developed program is proven to be useful for the data analysis of ACTAR signals. First experience using a program R3BRoot for the combined data analysis of the active target data together with the rest of R3B system is obtained. The algorithm of the time determination using ACTAR signals is developed. The comparison of leading-edge, CFD discrimination and slope fitting is done.

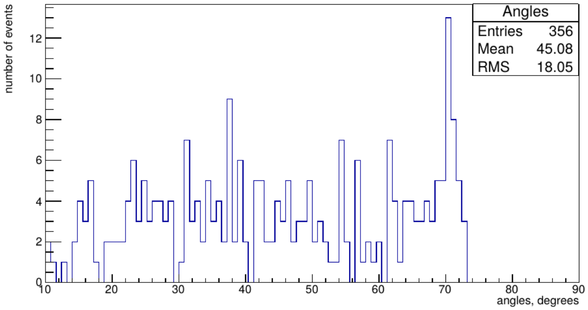

Fig. 1. The angle distribution.

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A Distribution Model for Fuels Production and Consumption in the World

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The exponential model of statistical distributions

$$f(n) = Ae^{\alpha n}$$

(n is the number ordering country) related to various fuels, namely gas, oil and coal and to production and consumption for world countries is studied. We found that the given exponential model fits better to known data compared with, for instance, gaussian distribution. The parameters of distribution vary from year to year. In our investigation we used the software package developed by I. Gorchakov [1] and Python 3.4.0 with libraries pandas and numpy (for data processing), matplotlib and seaborn (for potting charts), Scipy.optimize.curve_fit (for square approximation).

Our results are presented as figures where on x-axis we numerate the countries arranged in increasing order of consumption or production of fuels and on y-axis production (consumption) of the corresponding fuel. The second part of results is plots with the dependence of the coefficient in exponential function on time (years). We hope that our analysis could be helpful in prognoses estimating future situation in the field.

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Quasiclassical Asymptotics of Solutions of Difference Equations on the Complex Plane

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We study the one-dimensional difference Shrödinger equation

$$\frac{\psi(z+h)+\psi(z-h)}{2}+\cos z\ \psi(z)=E\psi(z),\ \ z\in\mathbb{C}, \tag{1}$$

where h is a fixed positive parameter and E is the spectral parameter. This equation appeared as a model for investigation of the spectrum of a Bloch electron in a crystal placed in a weak magnetic field.

Harper's equation (1) is typically quasiclassical:

$$\left(\cos\frac{h}{i}\frac{d}{dz}+\cos z\right)\psi(z)=E\psi(z),$$

i.e., we have small parameter h in front of the derivative.

V. Buslaev and A. Fedotov studied quasiclassical asymptotics of solutions of Harper's equation on the complex plane [1]. It turns out that solutions have the *standard quasiclassical behavior* for sufficiently small h on certain *canonical* domains on the complex plane.

We generalize this result to the case where the potential is a trigonometric polynomial and simplify the proof using ideas from the paper by A. Fedotov and F. Klopp [2].

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Specificities of Spin-Flop Transitions in Antiferromagnets with Two Types of Anisotropy

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We have considered the work "Switching of anisotropy and phase diagram of the Heisenberg square-lattice S=1/2 antiferromagnet $Cu(pz)_2(ClO_4)_2$" [1].

There was made a suggestion in this paper, that a constant of anisotropy changes it's sign in case of spin-flop, but we assume, that vector of magnetic structure changes it's direction. Using a phenomenological theory we have considered how changing of the direction of the magnetic field impacts on the reorganization of ground state of easy-axis antiferromagnet near the spin-flop region.

We have obtained an equation that determines two astroids. Within these astroids metastable states can exist. Reorientation of magnetic moment originates with the change of value of magnetic field directed along easy direction because of spin-flop.

We have tried to reproduce values of the critical angles. We have used the model of biaxial antiferromagnet, which was used in Smirnov's paper for interpretation of EPR spectrum. We have obtained the result that demonstrates that this model doesn't describe this compound.

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Generalized Two-Point Tree-Level Amplitude jf-> j’f’ in a Magnetized Medium

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The tree-level two-point jf-> j’f’ 0, where f is a fermion and j is a generalized current, in a constant uniform magnetic field of an arbitrary strength and in charged fermion plasma, for the jff interaction vertices of the scalar, pseudoscalar, vector and axial-vector types have been calculated. The generalized current j could mean the field operator of a boson, or a current consisting of fermions, i.e. the neutrino current. The particular cases of a very strong magnetic field, and of the coherent scattering of the real fermions without change of their states (the «forward» scattering) have been analysed. The contribution of the neutrino photoproduction process to the neutrino emissivity has been calculated with taking account of a possible resonance on the virtual electron.

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Avalanche to Streamer Transition Near in the Vicinity of a Spiral Electrode

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The phenomenon of avalanche-streamer transfer (AST) in air is considered. It occurs upon application of sufficient strong electric field to gases. The condition of streamer's initiation is formulated as the critical value of ionizing collisions committed by electrons on a certain electric field line. Streamers' formation easily leads to breakdown.

The Matlab program (using link with the Comsol Multiphisics software package) based on AST method is written for computation of breakdown voltage on the spiral electrode. The dependence of the breakdown voltage on the spiral's stretching degree is obtained. The both complete 3D model and approximate 2D formulation are analyzed.

The limits of applicability for 2D formulation are obtained. The permissible spiral's stretching range is established.

Relativistic Calculations of the Ionization Probabilities for a Many-Electron Atom Exposed to a Strong Laser Field

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The set of the time-dependent Dirac-Kohn-Sham equations for a many-electron ion exposed to a strong laser field is considered. The "frozen-core" model studied as the first step. Ionization probabilities for a many-electron ion were calculated and compared with ones previously calculated with other techniques.

At first stage the stationary problem was solved using the dual kinetic-balance (DKB) approach [1] and then the time-dependent problem for a hydrogenlike ion in presence of a strong electromagnetic field was solved using different propagation schemes: the Crank-Nicolson propagation scheme [2], split-operator technique [3], and Lanzcos propagation scheme [4]. The interaction with the electromagnetic field was considered within the dipole approximation.

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Optimal Operation Settings for the Low-Energy Injection System of CRYRING

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CRYRING is a heavy ion storage ring, a part of Facility for Antiproton and Ion Research (FAIR) at the GSI in Germany. It is currently under construction. The first part of the low-energy injection beamline of CRYRING is built to transport charged particles from the ion source to the RFQ (Radio Frequency Quadrupole). We identify the optimal voltage settings of two ion optics elements, namely the einzel lens and the quadrupole doublet, in order to minimize beam loss and to characterize the ion source. Optimal settings were found in experimental tests, as well as in a series of simulations with different voltages. Beam emittance in the horizontal plane is estimated both from the experiment and the simulation.

Settings		Optimal voltage, V	Estimated emittance
Experiment	Einzel lens	6550 ± 30	7 π*mm*mrad
	Quadrupole doublet	300 - 500	
Simulations with SIMION	Einzel lens	6850 ± 50	9 π*mm*mrad
	Quadrupole doublet	300	

The Program Complex for Cross-Compiling of Models of Virtual Laboratories in Physics to Android Platform

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BARSIC (Business And Research Interactive Scientific Calculator) is [1] domain-specific programming language [2]. The most important BARSIC applications are virtual laboratories in physics which are used in Online Contest in Physics (“Internet-Olympiad” in Physics). Online Contest provide a unique opportunity for testing of the practical application of student knowledge. This is achieved by means of models of virtual laboratories in Physics, simulating a real physical experiment. BARSIC is a software suite provides advanced graphics and mathematical capabilities, developed for mathematical simulation. Online Contest in Physics reached high attendance - about 40 thousand participants per year, and is held annually in more than 20 countries. However, its further development is limited by the BARSIC runtime, which can run now on MS Windows and Linux platforms only.

However, user can not run models of virtual laboratories on a number of platforms of popular operating systems (Android, iOS). Applications for Android platform are usually written on Java programming language. Java source codes it is necessary compile to the byte codes of the Android virtual machine (Dalvik or ART). It is possible re-write source codes of virtual laboratories on Java programming language [3]. However, this re-writing is very time consuming and costly. Moreover, it does not guarantee proper operation of the models. We have developed a prototype of the program complex for cross-platform compilation of source codes written in BARSIC programming language to Java source codes, Java byte codes and the byte codes for the Android platform. Architecture of the program complex gives it possible to extend target cross-compiled codes to Objective C codes for iOS platform. This approach makes it possible to guarantee the correct operation of the models of virtual laboratories compiled for different target platforms.

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H. Biophysics

Effects of Mg 2+ Ion Binding on the Secondary Structure of Bovine Serum Albumin

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We study the conformational properties of BSA, one of the most common plasma proteins responsible for several physiological roles and transport in particular. BSA is known to bind metal ions, such as Ca^{2+} and Zn^{2+} [1]. This suggests that the stability of a BSA molecule may be influenced by binding metal ions. Our goal is to evaluate the effects of the presence of Mg^{2+} ions on the secondary structure of BSA under conditions close to physiological. We use IR spectroscopy in D2O solution as a sensitive method allowing to distinguish between several structural elements (alpha-helix, beta-turn, beta-sheet). Analysis of amide I band (1600 – 1700 cm^{-1}) provides relative contributions from these secondary structure. We use $MgCl_2$ salt and explore the range of relative concentrations [Mg]:[BSA]= 1:5, 1:3, 1:1, 3:1 and 10:1, to be compared to salt-free BSA solution. The main result of this work is that the BSA secondary structure is quite stable and essentially unaffected by the presence of Mg^{2+} ions, see Fig. 1.

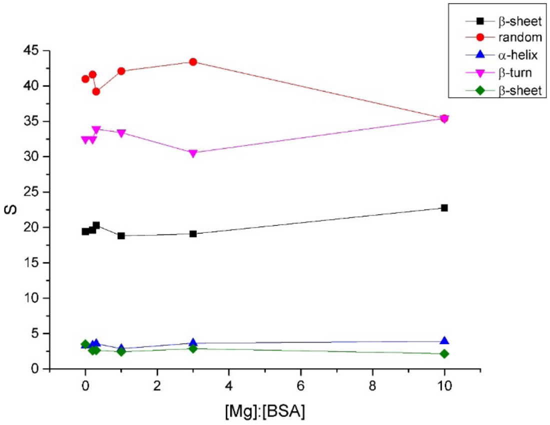

Fig. 1. Areas of the resolved absorption peaks, S, attributed to various secondary structure elements (indicated in the legend) vs. the relative Mg/BSA concentration.

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Computer Simulation Study of Structural and Dynamic Properties of DNA-lipid Complexes

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Formation of supramolecular complexes of DNA and zwitterionic phospholipids is important from the point of view of the development of non-toxic gene delivery vectors and DNA-based nanodevices interacting with cell membranes. While experimental studies have shown that divalent cations can promote adsorption of negatively charged double helixes of DNA on zwitterionic (neutral) phospholipid membranes, the underlying molecular mechanism of such adsorption as well as the microscopic structure of the resulting supramolecular DNA-membrane complexes are still unknown. To address this problem, here we employ atomic-scale molecular dynamics simulations to probe interactions between DNA and phospholipid bilayer membranes in aqueous solution with and without $CaCl_2$ salt. The state-of-the-art atomistic force-fields AMBER parmbsc0 and AMBER Lipid14 were used to describe a double helix of DNA and phospholipid molecules, respectively. We carried out microsecond-long molecular dynamics simulations which allowed us to evaluate a wide range of dynamic and structural characteristics of DNA-membrane systems. Overall, our results provide compelling evidence that Ca ions are largely responsible for attractive interactions between DNA and phospholipid membranes on a nanoscale: We demonstrate that divalent calcium cations serve as stitches between phosphate groups of DNA and lipid molecules, stabilizing thereby DNA-lipid complexes.

The simulations were performed on the Lomonosov supercomputer at the Moscow State University and on the computer cluster of the Institute of Macromolecular Compounds RAS. This work was partly supported by the Presidium of the Russian Academy of Science through the grant program ”Molecular and Cellular Biology” and also by the Russian Foundation of Basic Research through Grant No. 14-03-01073.

DNA Interaction with KE and KEDW Peptides

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It is widely known that short peptides, which are consisted of some amino acid residue, act as signaling molecules and take part in biological processes regulation. The peptides KE and KEDW were produced by using a basic method of peptide synthesis in a solution.

Clinical animal tests have shown the high level of immune and reparative activity. Furthermore, the experiments with cellular cultures of lymphocytes' cells have shown a great immune stimulating effect of KE which appears by the strengthening the activity of T helper receptors. KEDW is a synthetic peptide created by analyzing the amino acid composition of polypeptides that have an insulinotropic effect. The experiments on animals and cellular cultures have shown that KEDW peptide facilitate the process of conversion the stem cells into the secretory cells of pancreatic islets. Therefore, the peptide makes the secretory tissue of pancreas regenerate.

But the assumed aim of peptides activity was their impact on DNA molecule. Thus the purpose of the research was studying the interaction of KE, KEDW peptides and DNA molecule in the solution. The research material was made by mixing the KE or KEDW with DNA molecule in 5 mM of NaCl. The using of KEDW peptide showed the reduction of amplitude and the offset of the maximum of the DNA absorption spectrum. KE peptide showed no modification in spectral properties of DNA in the solution.

For the research of the peptides impact on tertiary structure of DNA the method of low-gradient viscosimetry was used. There were some results of measuring the viscosities of the DNA solutions which contained various amounts of peptides. Those results showed the peptides influence on the tertiary structure of macromolecule.

In order to prove that interaction of peptides and DNA molecule can change its rigidity, we used the birefringence method that helped us to determine optical anisotropy of the statistical DNA segment which most probably depends on the molecule's rigidity. In this case there was detected the 15-20% decline of optical anisotropy for each peptide and this fact was a verification of our hypothesis.

The summation of experimental data gives us a right to conclude that KE and KEDW peptides have a bond with DNA molecule and they have an impact on the tertiary structure of macromolecule. Furthermore, there is a hypothesis that the amino acid the tryptophan causes all the modifications in the data gained by spectrophotometry method. And it means that this amino acid directly takes part in the forming of the research material.

Study of Silver Ions Binding to DNA and the Problem of DNA Metallization

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DNA interaction with silver ions have been studied earlier. In our days the interest to a detailed consideration of DNA-Ag+ complexes caused by the needs of modern technology using DNA as a template to create different nanostructures for medical, nanoelectronic, nanooptic applications. DNA can be used not only as a main biological polymer, but also as a convenient material for the manipulation in nanotechnological developments.

Silver ions can interact with DNA via the electrostatical attraction to phosphates or due to the formation o0f coordination bonds to heterocyclic nitrogen atoms of base pairs. We examined DNA solutions with different concentrations of Ag+ by spectral methods. It was shown that there are two different types of spectral changes after DNA binding with silver ions. At low Ag+ concentrations the hypochromic effect with the red shift of the maximum of DNA absorption band is observed. At higher Ag+ concentration the hyperchromism arises as a result of destabilization of DNA secondary structure.

After the formation of DNA-Ag+ complexes the DNA metallization with the addition of reductive agents was performed. The appearance of silver nanoparticles in DNA solution was checked by the emergence of plasmon resonance peak in the absorption spectra. The obtained results for the different DNA and Ag+ concentrations were analyzed. Conformational changes of DNA molecule in complexes with Ag+ and after the metallization were regarded.

Velocity Sedimentation as a Tool for Investigation of the Molar Mass Distribution of Polymer Systems. New features

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The molecular mass distribution and the degree of polydispersity are among the main characteristics of polymer samples. The degree of polydispersity is usually characterized by the Mw/Mn ratio.

The approach was presented to quantitative estimation of polymer samples' polydispersity from velocity sedimentation data using the Sedfit cluster. This approach is common for different classes of polymers. In this work it is demonstrated by the sedimentation data for statistical copolymer of N-methyl- N-vinylacetamide and N-methyl-N-vinylamine hydrochloride (MVAA–MVAH). Fractions of the copolymer with the average composition of samples 95.6:4.4 mol.% were obtained by the hydrolysis of homopolymer poly(N-methyl-N-vinylacetamide) (PMVAA) with HCl. Homopolymer PMVAA was investigated earlier [1]. The study was carried out in 0.2M NaCl solution, i.e. in conditions when polyelectrolyte effects were suppressed. Methods of molecular hydrodynamics, such as velocity sedimentation, translational diffusion, and viscometry, were used. The absolute molar masses and Kuhn-Mark-Houwink-Sakurada relations for intrinsic viscosity, sedimentation and translational diffusion coefficients in 0.2M NaCl solutions were obtained. The velocity sedimentation of the polyelectrolyte solutions in 0.2M NaCl solvent was studied with a Beckman XLI analytical ultracentrifuge in a two-sector cell with the optical path length of 12 mm at the rotor speed of 40 000 rpm. The sedimentation interference scans were processed with Sedfit program [2].

Sedfit is the cluster of programs which includes various processing of sedimentation scans. The concentration dependence of sedimentation coefficient was taken into account using Gralen equation. Distribution dc/ds (s) was converted to dc/dM (M) distribution and then molar masses Mw and Mn were estimated from dc/dM (M) distribution.

Acknowledgements. The polymers were synthesized in the Laboratory of hydrophilic polymers of the Institute of Macromolecular Compounds. Authors are very thankful to the Head of laboratory, Corresponding Member of RAS, Prof. E.F. Panarin and to the scientific researcher I.I. Gavrilova.

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Reduction of Silver Ions on DNA and Small Interference RNA: a Transition from Clusters to Nanoparticles

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Reduction of silver ions on DNA and siRNA attract an attention of scientists due to the possibility of creating sensors, biochips, etc. The usage of nucleic acids in new technologies as a matrix for creating several nanostructures with unique optical properties is interesting for creating devices and structures of several applications e.g. nanoelectronics, nanophotonics, information technology, etc. The solid metallization or "mosaic" metallization of polymeric chains can be carried out. The luminescent clusters may be useful for the construction of luminescent labels for bioimaging.

The goals of this research were to develop the method of creation of luminescent silver nanoclusters on siRNA and to compare the results with those for the luminescent clusters on DNA. The additional aim of the research was to apply the method of the synthesis of silver nanoparticles of several shapes with the plasmon peaks in visible spectral region for the metallization of DNA in a solution. The method of the reduction of silver ions after their binding to DNA was used as an alternative approach to form silver nanoparticles on DNA strands.

It was shown that the luminescence of Ag-siRNA and Ag-DNA complexes occurs in the same spectral region. Maximum of the luminescence band for Ag-DNA clusters undergoes a permanent bathochromic shift with the increasing of excitation wavelength. In contrast to this, luminescence of Ag-siRNA clusters produces only two intensive bands. This fact points on the smaller variety of Ag-siRNA luminescence clusters in contrast to Ag-DNA. The excitation at λ_{ex}=270 nm within the absorption area of nucleic acids shows very broadband luminescence spectrum for Ag-DNA solution, i.e. all types of nanoclusters are exited. When the long-wave excitation at λ_{ex}=600 nm in Ag-siRNA is used the luminescence in not observed in contrast to the significant luminescence for Ag-DNA clusters at the same λ_{ex}.

When nanoparticles are formed on DNA after the preliminary binding and reducing of silver ions, the spherical nanoparticles are observed directly on DNA strands, whereas the nanoparticles of triangular shape on the substrate may be not associated with DNA.

Conformational Transitions in an End-Grafted Chain Admixed to a Polymer Brush Made of Starlike Macromolecules

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An end-grafted single polymer chain inserted into a planar brush made of arm-grafted starlike macromolecules is studied theoretically by using the Scheutjens-Fleer self-consistent field method. Effect of the grafting density (number of grafted stars per unit area), the number of star arms, and the length of the linear chain on the chain conformation is investigated. We show that a chain shorter than the “longest path” in the star (equal to double arm length) acquires a coil conformation close to the grafting surface, at any grafting density. A chain which length exceeds the “longest path” length can undergo a transition from the coil to the “flower” conformation consisting of an extended "stem", immersed into the brush connected to a coil-like “crown” on the top of the brush. This transition is the first-order-like transition: it occurs sharply, and a coexistence of two states ("coil" and "flower") is observed in the transition region, this is expressed via bimodal shape of the chain end distribution. The coil-to-flower transition can also be induced by increasing the chain length provided that the grafting density is fixed. In dense brushes this transition is also the first-order-like whereas in loosely grafted brushes it occurs continuously without co-existence of two states. Such a continuous transition is characteristic for a chain inserted into the brush of linear macromolecules. It is shown that the length of the chain at the first-order transition point is a decreasing function of the grafting density, that is, it decreases with increasing thickness of the brush.

Acknowledgments

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Hydrodynamic and Conformational Properties of Poly(phenylene) Pyridine-Containing Hyperbranched Polymers in Solution

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Pyridyl(phenylene) hyperbranched polymers have a high rigidity, high solubility, low viscosity, chemically and thermally stable. Therefore, investigation of characteristics of the hyperbranched polymers has raised researcher's interest.

This paper reviews behavior of pyridinephenylene-containing hyperbranched polymers in solution by using methods of viscosimetery, densitometry, refractometry, high-speed sedimentation, dynamic light scattering, flow birefringence. There were determined values for these objects such as refractive index increment, sedimentation constant and coefficients of diffusion. These data has let to find out molecular weight and hydrodynamic invariant values. Optical shear coefficients and optical anisotropy were also calculated.

Computer calculations of parameters for studied objects (diffusion coefficient, hydrodynamic radius, sedimentation constant, intrinsic viscosity) were made in the specialized program HYDRO [1]. All the structure conformations were previously processed by molecular dynamics in program package HyperChem. Computations of hydrodynamic radius, intrinsic viscosity and diffusion coefficient of the structures were produced for two limited cases of conformations ("stick" and "sphere"). Previously conformations built in the program HyperChem.

The comparison of the hydrodynamic characteristics is obtained from experiment and computer calculations.

Acknowledgments

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Hydrodynamic Properties of Poly(phenylene) Pyridine-Containing Dendrons of Second and Third Generations in Solution

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The combination of structural symmetry of dendrons and possibility of modification of the terminal groups is the base for development of functional nanoscale materials with unique electronic, optical and magnetic properties. Due to presence of pores and voids in the structure of these polymers, it can be used in medicine as a corpuscular nano-carrier.

The paper investigates behavior of the pyridinephenylene-containing dendrons of second and third generations with aliphatic end groups ($C_{12}H_{25}$) and without them in benzene solution. Features of objects were studied by methods of molecular hydrodynamics: viscosimetery, densitometry, refractometers, high-speed sedimentation. Also, there were obtained values of the intrinsic viscosity, diffusion coefficients, with the partial-foot volume and sedimentation constant. The molecular mass and hydrodynamic invariant were calculated for both generations.

The comparison is made for experimental results with the computed data for hydrodynamic characteristics (intrinsic viscosity, diffusion coefficients and sedimentation constant) of investigated dendrons that are obtained by computer calculations in scientific program HyperChem and HYDRO [1]. All the structure conformations were previously processed using molecular dynamics in program package HyperChem.

The analysis of computational and experimental hydrodynamic characteristics of the dendrons with aliphatic end groups and without them has been held.

Acknowledgments

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Structure and Properties of Polymer Brushes Made of Arm-Grafted Polyelectrolyte Stars: a Theoretical Study

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Polymer brushes are the monolayers of polymer molecules densely grafted onto an impermeable surface. They are used for surface modification in order to improve their barrier properties or biocompatibility. In recent years, brushes formed by regularly branched macromolecules, in particular, dendrons and stars, attract a lot of attention.

The present work is devoted to theoretical study of the planar brush formed by arm-grafted polyelectrolyte stars. The system was investigated by using the Scheutjens-Fleer self-consistent field (SCF) numerical approach. The case of a strong polyelectrolyte star with fixed charge distribution at high and low salt concentration was considered. The effect of grafting density, number of star arms, and the degree of ionization on the brush properties was investigated. It was shown that with an increase in the grafting density, the number of arms, and the degree of ionization arms leads to the increase in the brush height and favors partitioning of stars into two “populations” with weakly and extremely strongly extended grafting arm, or “stem”. A comparison of the SCF modeling results with the predictions of scaling theory for the brush height was made. A good agreement was observed for loosely grafted brushes where the electrostatic interactions in the brush dominate over the excluded volume interactions.

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FTIR Investigation of Alpha-Keratins in Biological Samples

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Fibrous proteins play a significant role in animals' organism. They are parts of supporting, forming, coupling elements (cartilages, tendons, bones) and of external protective covers (wool, feathers, shell). Mechanical characteristics of these proteins are determined by their structure: water-insoluble supramolecular formation of parallel to each other oblong polypeptide chains [1]. The same structures are arisen in a tissue at prion diseases. They consist of infected isoform of prion proteins united into large fibre and later into an amyloid plagues, resistant to the proteases and denaturants [2].

IR spectroscopy is a very promising method for the molecular structure analysis. Particularly it helps us to get information about the protein secondary structure and their conformational transitions. Investigation of different fibrous proteins structure can help us to understand a mechanism of prion fibrils formation and their possible destruction.

We received IR-spectra of chicken plumage, human nails and hair pounded and pressed with KBr in tablets. In every spectrum we've got the Amid I band was considered, 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 [3]. The decomposition to Gaussian contours components was applied. We've got the content of α-helices close to 50% for each protein studied. It agrees with data for alpha-keratins from other biological samples [4]. It is worth to notice that even the soft extraction of alpha-keratin from the wool results in the distortion of the protein structure: the decrease of α-helices content and the raise of β-sheets and disordered structures occur [4].

The research was performed at the Center for Optical and Laser Materials Research of Research park of Saint Petersburg State University.

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Surfactant-Based Vector for the Delivery of Small Interfering RNA

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Inducing specific gene silencing, molecules of small interfering RNAs are a promising drug for gene therapy. A carrier is required to deliver the nucleic acid through the cellular membrane and also to protect it from rapid degradation in biological systems. Cationic surfactants, whose micelles neutralize negative charge of nucleic acid molecules, are yet poorly investigated as delivery agents. We tested the cationic surfactant AzoTAB as an agent that can form nanocarriers for the delivery of siRNA. The delivery was studied by fluorescent microscopy. The conditions (concentrations, charge ratio, ionic strength of the solutions), upon which the nanocarriers are formed, are determined. Earlier, they were determined for DNA – surfactant systems in our study [1].We obtained information of the size of nanostructures formed upon varied charge ratios $z = C(\text{AzoTAB})/C(\text{siRNA})$ using atomic force microscopy and dynamic light scattering. Values of zeta potential were measured for nanostructures. We also focused on binding of the surfactant to siRNA, it was investigated by fluorescent spectroscopy.

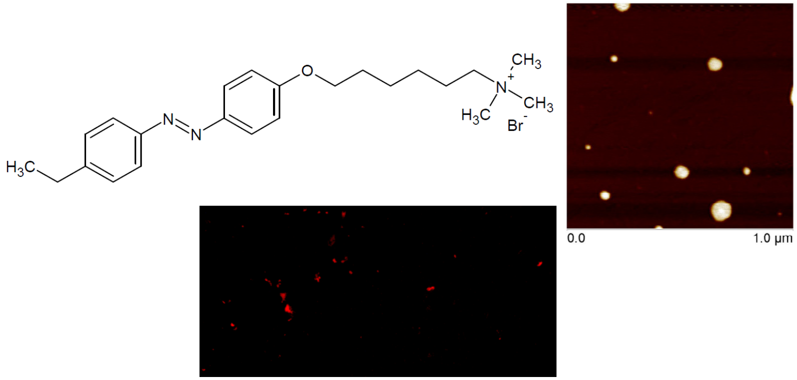

Fig. 1. Structure of AzoTAB, nanostructures (AFM image) and cell delivery (fluorescence image).

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I. Resonance Phenomena in Condenced Matter

Characterization of Building Materials with NMR Relaxation

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Cyclic changes in temperature can have a significant impact on the structures of concrete and ceramics. In periodic freezing and thawing of the fluid in the pores of the structure of the pore space can vary, which affects the strength characteristics of the materials and may ultimately determine the "lifetime" of the construction or product. The aim of this study is to explore the influence of cyclic freeze samples of porous ceramics and concrete, which are saturated with water, on the relaxation characteristics of the nuclear magnetic resonance. The relevance of this study confirms the possibility of using its results for the analysis of frost resistance of building materials.

In the course of this work was studied the effect of cyclic freezing water-saturated porous samples to NMR relaxation characteristics. According to the results of the experiment revealed a number of dependencies, which carry the following information:

- The dependence of the relaxation times of the rooms freezing cycle allowed us to determine that connectivity has changed during the experiment.
- Changing the relative content of components shown, the number of macropores increased, indicating that the changes in the structure of the sample after 60 cycles of temperature change.
- The experiment was based on deuterium water saturated samples showed that the presence of paramagnetic centers on the pore surfaces has not significantly effect on the relaxation.

A Complimentary Study of the Ddisordered $Fe_{0.92}V_{0.08A}$ Alloy via ^{51}V NMR and DFT

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There is an increasing interest in Fe-V systems in scientific and industrial areas. The systems demonstrate a number of exceptional magnetic properties. Although the bulk vanadium is non-magnetic, while being in bcc $Fe_{1-x}V_x$ alloys with $x \leq 0.2$ it is polarized and exhibits an induced magnetic moment up to about 1 μB [1-3] for x close to 0. Moreover, magnetic moments of Fe and V atoms are always coupled antiferromagnetically. The magnetic polarization of V atoms was also observed in other Fe-V compounds, such as $Fe_{3-x}V_xX$ (Si, Ga, Al) and $RFe_{12-x}V_x$ (R = rare earth atom). Among them bcc $Fe_{1-x}V_x$ is the most convenient object as its relative simplicity allows us to develop new methods for studying such kind of materials.

Magnetic properties of $Fe_{1-x}V_x$ alloys were studied by different methods including polarized neutrons [1], x-ray magnetic circular dichroism (XMCD) [2] and theoretical methods [3]. Although neutron diffraction detects magnetic moment in a certain crystallographic site, it does not identify to which atom (Fe or V) it is associated. XMCD, in its turn, provides information about magnetic polarization of a selected atomic shell, but it is not site-resolved. From this perspective nuclear magnetic resonance (NMR) is a powerful tool, which allows us to record both atom and site-resolved V signal. However, in order to evaluate the influence of V atom encirclement from NMR spectra it is necessary to make computer calculations.

In this contribution we report on the result of our complimentary study of the magnetic properties and vanadium atom distribution in the $Fe_{0.92}V_{0.08}$ experimentally by ^{51}V NMR and theoretically by density functional theory (DFT) combined with Monte Carlo simulation.

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The NMR Relaxation and Molecular Dynamics of the Ionic Liquid (Ethyl-Octyl Imidazolium Chloride) in Aqueous Glycerol Solutions

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Ionic liquids (IL) are often referred to as organic compounds consisting of a cation and an organic or non-organic anion, having a melting point below 100°C. Cations determine the physical properties of IL (melting point, viscosity, density), whereas anions determine chemical properties. Since the physical and chemical properties of ILs properties can be adapted to the specific conditions by careful selection of cations and anions, IL became widely used in a variety of scientific and industrial applications [1].

This research is a part of a program devoted to the study of the effects of glycerol on the micellization of IL in aqueous solutions that is of great interest for cosmetology, pharmaceuticals and other industries [2]. The significant work in this research has been undertaken and the results are summarized in the present paper.

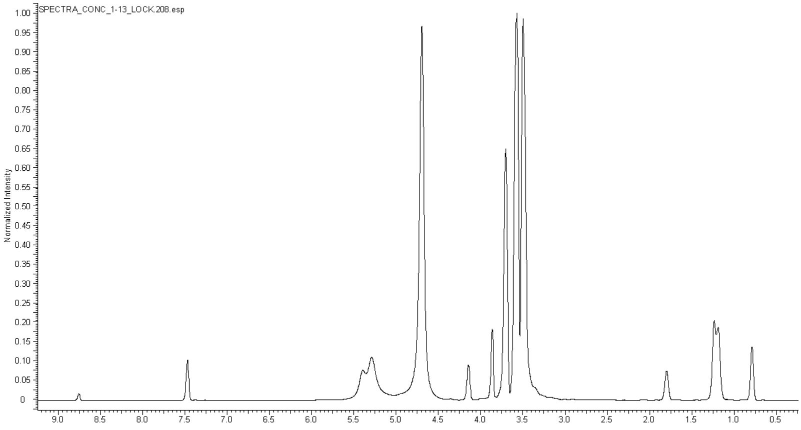

Fig. 1. 1H-NMR spectrum of IL in aqueous glycerol solution.

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Diffusion Weighted NMR Imaging at 7 mT

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The special feature magnetic resonance imaging (MRI) is a possibility to visualize varies characteristics of investigated object. Among others a peculiar interest represents a mapping of spatial distribution of self-diffusion coefficient. A high water content in the human organism permits to use this ability as diagnostic technique in medicine. Diffusion weighted imaging (DWI) is rather new effective versions of MRI. As a rule, such images are obtained with medical magnetic resonance scanners at high magnetic field (1-3 T and more) [1].

The technique of DWI allows us to construct a map of molecular diffusion rates (as a rule, water molecules) in biological samples. The features of water molecules diffusion can reflect a state of biological tissues.

Magnetic resonance imaging in very low field more and more becomes widespread subject of research [2, 3]. In this report the results of experiment on obtaining DWI at magnetic field 7 mT are presented, using the laboratory homebuilt nuclear magnetic resonance imager in department of Nuclear-Physical Research Methods. For realization of the imaging pulse sequence the special program was created in the LabVIEW environment.

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Simulation of Mapping of Static Magnetic Field Using Magnetic Resonance Iimaging Technique

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Homogeneity of the field plays a very important role not only in Nuclear Magnetic Resonance but Nuclear Magnetic Tomography also (spectral and spatial resolving capacity).

Methods of getting Magnetic Resonance images can possibly fit to getting fast and convenient spatial distribution of the magnetic field in a workspace of the spectrograph or tomograph.

The purpose of my work is to clear up particular features of one of the methods of getting spatial distribution of the magnetic field presented in [1]. The difference of this method is that except inverting (180 impulse) radio-frequency impulse, there is also the bipolar gradient impulse, which is used for getting gradient echo. As a result combined echo appears after the time of (2T+τ) but not after 2T as normal radio-frequency spin echo.

For that purpose numeral simulation was realized with different spatial distributions of the magnetic field.

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2D NMR Spectra Fitter

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NMR spectroscopy is a powerful tool of scientific research. It helps to obtain information about the studied material on the molecular and atomic levels without destroying the sample. The obtained data from the NMR spectrometer can be then analyzed using different data analysis packages to get important molecular properties of the sample. Those packages, although available and not so hard to use, are written on non-popular programming languages. Matlab, on the other hand, is a popular numeric computing environment amongst young scientists, yet it doesn't have a comfortable means of spectra fitting and analysis. The need to use Matlab for 2D NMR spectra fitting is the motivation for this work.

"2D NMR spectra fitter" is a toolbox [1] that allows the researchers to fit 2D spectra and obtain their useful parameters such as peak width. After the NMR signal is obtained, a Fourier transform gives us a spectrum that consists of Lorentzians and Gaussians. 1D NMR spectra can be used to obtain a lot of useful information about the atoms, but it suffers from peak overlapping when system studied is not trivial. 2D NMR spectra allow overcoming this discrepancy and can be used, for example, to study a protein's structure. Homonuclear and heteronuclear NMR experiments are good examples of this approach.

Our toolbox uses as input two files: one that has spectrum data and one that has peaks' coordinates. As an output it provides a table of fitted peaks' parameters. It imports data from the files into Matlab. To fit 2D spectrum we either need to fit all the peaks at a time and thus spend too much time waiting for the results or we need to fit the spectrum as separated peaks and thus we will not have correct results for partially overlapping peaks. So we had to find an algorithm that can save both time and accuracy.

Such algorithm starts with dividing the spectrum into clusters of close-positioned peaks and then fits each cluster separately. The clustering part of the algorithm starts with each peak at a time, checks whether it has in vicinity other peaks or not, builds a cluster that includes those peaks and returns a matrix that contains each cluster's center, dimensions and the number of peaks that it includes. The toolbox fits the peaks with 2D Gaussians and then moves on to fit the next cluster. It returns a matrix that contains each peak's center, width and the calculation uncertainty.

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Study of Hydrogen Mobility in the Lattice of Ternary Ti-V-Cr Intermetallics for Hydrogen Storage Using NMR Techniques

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The ever-increasing power consumption calls for searching for clean and renewable energy sources. Hydrogen offers environmentally friendly and efficient alternatives to the combustion of gasoline and other fossil fuels. However, its storage in pure form is energy-consuming. The most energy-optimal solution of the hydrogen storage problem is to store it in a bound state, for example, in a metallic lattice as a hydride.

Transition metal alloys (Ti-V-Cr) exhibit low temperature of the hydrogen desorption (which can be changed by the alloy composition) and rather high hydrogen sorption kinetics. Sorption properties of the systems can be improved by the addition of a minor fraction of Zr_7Ni_{10} [1]. It is particularly interesting to study this addition because individual hydrides of two-component alloys have fast hydrogen kinetics and are not soluble in the main alloy that results in the two-phase structure. Main alloy (Ti-V-Cr) crystallizes into the bcc structure in a wide range of composition. During hydrogenation a bcc→fcc phase transition occurs.

Sorption properties of hydrides depend on the activation energy (E_a) of hydrogen motion in the lattice. Hence, study of a large number of alloys with variety mass fraction is an important task for making a conclusion about the impact of the substance on the kinetics of hydrogen in its technique.

Nuclear magnetic resonance (NMR) has approved itself quite valuable for studies both the hydrogen location and mobility in metals. The activation energy of hydrogen mobility in the lattice of ternary Ti-V-Cr can be determined using two different techniques of NMR: from proton spin-lattice relaxation experiments and the hydrogen diffusion coefficient measurements.

All hydrides exhibit rather slow hydrogen diffusion ($D = 1\div3\times10^{-11} m^2/s$). The activation energy (E_a) strongly depends on the composition of the studied compound. For the Cr poor hydrides with fcc structure the E_a values, obtained from both relaxation and diffusion measurements, are in fair agreement.

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S. First Steps in Science
(for secondary school students)

Silver Nanoprisms and their Properties

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The paper presents the results of a study of silver nanoprisms synthesized by means of silver nitrate reduction using potassium bromide.

$$NaBH_4 + 8AgNO_3 + 4H_2O \leftrightharpoons Na[B(OH)_4] + 8Ag + 8HNO_3$$

Four colloidal solutions containing silver nanoparticles have different colors depending on the volume of KBr added to the solution, the KBr affecting the particle size. The higher the concentration of KBr in the solution, the smaller the nanoprisms.

The solution absorbance study results confirm the influence of KBr on nanoprism size. The higher the concentration of KBr in the solution, the higher the solution absorbance. A transmittance study has shown that the higher the concentration of KBr in the solution, the greater the probability of sprectral matching for the metal core and metal sheath plasmon resonance peaks. That effect depends on the nanoparticle shape which in turn is influenced by the Kbr concentration. Researching SERS-activity (Surface-enhanced Raman spectroscopy) has shown that all colloids increase SERS-activity, and some of the solutions have increased SERS for more than ten times.

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