

CONFERENCE ABSTARCTS

International Student Conference

“Science and Progress”

DAAD

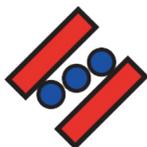


Санкт-Петербургский
государственный
университет

Freie Universität



Berlin



German-Russian
Interdisciplinary
Science Center

St. Petersburg – Peterhof
November, 10-14
2014

Organizing Committee

Prof. Dr. A.M. Shikin,	G-RISC Coordinator, SPSU
E.V. Serova,	Administrative coordinator of G-RISC, SPSU
M. Rusinova,	G-RISC office, SPSU
T. Zaliutdinov,	G-RISC office, SPSU

Program Committee

Prof. Dr. E. Rühl,	G-RISC Coordinator, FU Berlin
Prof. Dr. C. Laubschat,	Faculty of Physics, TU Dresden
Prof. Dr. A.M. Shikin,	G-RISC Coordinator, SPSU
Prof. Dr. V.N. Troyan,	Faculty of Physics, SPSU

Contacts

Faculty of Physics, Saint-Petersburg State University
Ulyanovskaya ul. 1,
Peterhof, St. Petersburg, Russia
198504

Tel. +7 (812) 428-46-56,
Fax. +7 (812) 428-46-55
E-mail: g-risc@phys.spbu.ru
office@g-risc.org
Website: www.g-risc.org

Heads of sections

- A. Chemistry** – Dr. A.A. Manshina,
Institute of Chemistry, SPSU
- B. Geo- and Astrophysics** – Prof. Dr. V.N. Troyan, Faculty of Physics, SPSU,
Prof. Dr. N.R. Ikhsanov,
Faculty of Mathematics and Mechanics, SPSU
- C. Mathematics and Mechanics** – Prof. Dr. S. Yu. Pelyugin,
Faculty of Mathematics and Mechanics, SPSU
- D. Solid State Physics** – Prof. Dr. A.P. Baraban,
Faculty of Physics, SPSU
- E. Applied Physics** – Prof. Dr. A.S. Chirtsov,
Faculty of Physics, SPSU
- F. Optics and Spectroscopy** – Prof. Dr. Yu.V. Chizhov,
Prof. Dr. N.A. Timofeev,
Faculty of Physics, SPSU
- G. Theoretical, Mathematical
and Computational Physics** – Prof. Dr. Yu.M. Pis'mak,
Faculty of Physics, SPSU
- H. Biophysics** – Prof. Dr. N.A. Kasyanenko,
Faculty of Physics, SPSU
- I. Resonance Phenomena
in Condensed Matter** – Prof. Dr. V.I. Chizhik,
Faculty of Physics, SPSU

Invited Lectures

XMCD: a Versatile, Element Specific Method for Studying Magnetism in Multi-Component Systems

Kai Fauth
fauth@physik.uni-wuerzburg.de

Physics Institute, University of Würzburg, Germany

First reported in 1986, x-ray magnetic circular dichroism (XMCD) has since been established as a spectroscopic tool for the investigation of magnetism. Being related to resonant x-ray absorption at core level thresholds, it is inherently element and orbital specific and capable of discerning spin and orbital contributions to magnetic moments. XMCD has thus greatly contributed to our contemporary understanding of magnetism in alloys and the mechanisms behind magnetocrystalline anisotropy. When detected by electron yield, it also reaches very high sensitivity, reaching into (sub-percent) fractions of an atomic monolayer.

The lecture shall introduce and review some basics of the method and illustrate some of its capabilities, emphasizing the combination of spectroscopy and spectroscopic “magnetometry”. Examples shall include isolated adatoms on surfaces, nanoparticles of magnetic alloys and the study of magnetic properties in heavy fermion systems.

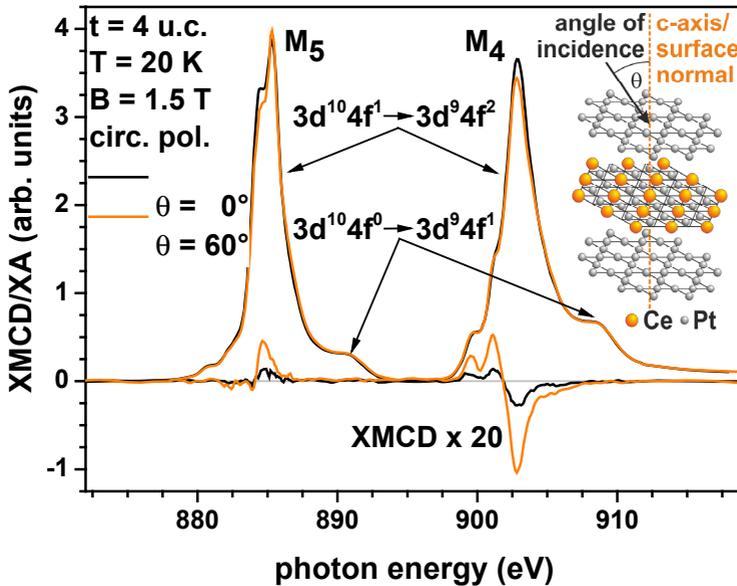


Fig. 1. X-ray absorption and magnetic circular dichroism spectra of a single crystalline thin film of CePt₅. Details of line shape and their variation with specimen orientation reveal important information on the electronic configuration. Most prominently, the Ce4f paramagnetic response is strongly anisotropic.

Electron spin polarimetry for spin resolved photoemission

O.E. Tereshchenko
teresh@isp.nsc.ru

*Novosibirsk State University, Novosibirsk, Russia Rzhanov Institute
of Semiconductor Physics SB RAS, Novosibirsk, Russia*

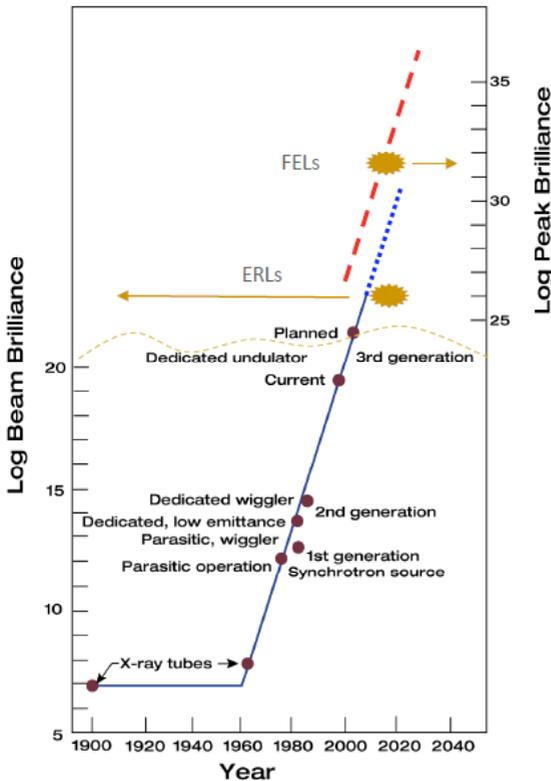
A new method of free electron spin detection has been realized by measuring the cathodoluminescence intensity from injected electrons into the Pd/Fe/GaAs/InGaAs heterostructures. This method is based on the measurement of the light emitted from the recombination of the spin-filtered electrons in the InGaAs quantum wells. The spin-filtering effect in the ferromagnetic thin layer induces the spin selectivity that allows a simple detection of the luminescence light intensity emitted from the semiconductor providing an asymmetry proportional to the incident electron beam spin-polarization. With respect to the analogue of electrical spin-detection technique in metal/semiconductor junctions, which gives comparable value of the figure of merit with a standard Mott polarimeter, optical measurement may provide significant advantages for a number of applications since it only requires to contact one of the two junction terminals, it is insensitive to the rectifying properties of the junction and it is compatible with photon counting techniques. Moreover, unlike structures where a light detector is integrated, such optical detection techniques could also allow the development of a 2D spin polarimeter for spin imaging applications. The optical spin-detector can be integrated into the registration channel of the hemispherical electrostatic analyzers with the possibility of simultaneously detecting of angular distribution and spin polarization of photoemitted electrons.

Synchrotron Radiation: Production, Properties, and Uses

Hartmut Zabel
harzabel@uni-mainz.de

*Department of Physics, Johannes Gutenberg University Mainz,
Germany*

Synchrotron radiation, discovered in 1947 by chance, has rapidly advanced in recent years to unprecedented brilliance which is exploited for the analysis of materials on the spatial scale down to nanometers and time scales as short as femtoseconds. More than 40 large synchrotron radiation facilities exist presently worldwide serving an increasing scientific and industrial community to explore with exceptional accuracy structural, spectroscopic, dynamic and kinetic questions ranging from biology, chemistry, and solid state physics to energy, civil engineering, and cultural heritage.



In this lecture I will provide an introduction and overview on synchrotron radiation, its production, properties, and the various applications. Starting with some fundamental properties of synchrotron radiation, the development from the early parasitic uses until the present fourth generation of free electron lasers will be briefly sketched. Some selected examples will illustrate the present analytical power that experiments with synchrotron radiation provide. The lecture will conclude with perspectives for new generations of synchrotron sources.

Taken from a lecture of George Srajer, ANL

German-Russian Interdisciplinary Science Center (G-RISC)

Prof. Dr. Eckart Rühl, Natalia Kolanovska
office@g-risc.org

The German-Russian Interdisciplinary Science Center (G-RISC) was founded as a binational platform of scientific research and education with two main offices at Saint-Petersburg State University, Russia and Freie Universität Berlin, Germany.

The Center of Excellence was established in March 2010. It builds on a long-standing tradition of scientific cooperation between scientists of Russia and Germany. G-RISC relies on funding and regulations of the German Academic Exchange Service (DAAD) and the German Federal Foreign Office. The Center supports education and research in binational projects between both countries. Focus is interdisciplinary research in four fields of natural sciences: physics, geophysics, physical chemistry, and mathematics.

G-RISC is operated by two scientific coordinators: Prof. Alexander Shikin (Saint-Petersburg State University) and Prof. Eckart Rühl (Freie Universität Berlin), supported by administrative coordinators and binational Steering Committee.

G-RISC encourages the experienced and novel promising groups to submit their projects. Proposals can be submitted by all research institutions in Russia and Germany and are selected by Steering Committee on the basis of their scientific quality. This type of competition is organized every six months. The next call for proposals runs from October 1, 2014 (deadline: October 31, 2014). In January 2015 starts the next funding period, provided funding is approved by the German Academic Exchange Service (DAAD).

G-RISC funds primarily mobility of young researchers between Russia and Germany. This concerns first of all research stays in laboratories of the partner groups in the other country. It is anticipated that research stays and stipends are strengthening stable long-term collaborations between Russian and German researchers. Each single project is important to tie researchers and research interests together and to develop novel, interdisciplinary projects between Russia and Germany.

In total, more than 75 institutions from Russia and Germany and more than 300 young and experienced researchers from Russia and Germany conduct research and teach at the Center. Since the opening of G-RISC 16 interdisciplinary workshops/conferences have been held with the support of the Center with more than 1000 participants.

Detailed information about the Center of Excellence can be found at the G-RISC website: <http://www.g-risc.org>.

Russian-German Laboratory at BESSY II, Berlin

Dmitry Marchenko Eckart Rühl
dmitry.marchenko@fu-berlin.de

Physikalische und Theoretische Chemie, Institut für Chemie und Biochemie, Freie Universität Berlin, Germany

The Russian-German Laboratory is one of the leading facilities for collaborations between Russian and German research groups in the field of structural research. It is located at synchrotron radiation facility BESSY II, Helmholtz Center Berlin, Germany. Seven research institutions from Russia and Germany support this binational laboratory, which is open to the international user community. About 30 groups come there to conduct experiments each year, publishing ca. 35 articles per year in peer reviewed journals. It is also a very powerful platform for students to get profound knowledge in advanced, novel equipment yielding excellent scientific results. These results are used for publications as well as Bachelor, Master, and PhD theses. The laboratory is tightly collaborating with the German-Russian Interdisciplinary Science Center (G-RISC), providing substantial support for those who are working in the Russian-German Laboratory.

The main part of the laboratory is the Russian-German beamline which provides easily tunable intense ultraviolet radiation and soft X-rays in a wide energy range. This allows one to study a large variety of physical, chemical, and biological phenomena, such as electronic and structural properties of organic or inorganic materials, nanostructures, biological systems, novel carbon-derived materials, and electron-correlated materials. There are several types of photoemission, absorption and electron diffraction techniques available for the research groups with state-of-the-art research environment and support.

The Russian-German laboratory is always in active development and upgrade process. At the moment the photoemission electron microscope is under commissioning and becomes available for users coming to the laboratory. Construction of the second beamline will start this year, which together with the new experimental station would double the number of visiting research groups, available techniques and realized projects. In this lecture we will consider the current state and the future plans of the laboratory in details, consider the research techniques and examples of scientific results, discuss the possibilities to visit the laboratory with your own projects.

Nonlocal Problems for Vlasov-Poisson Equations with External Magnetic Field in Infinite Cylinder

Alexander Skubachevskii
skub@lector.ru

Peoples' Friendship University of Russia, Moscow, Russia

The Vlasov-Poisson equations in infinite cylinder describe the evolution of density distribution functions for charged particles of high-temperature rarefied plasma in mirror trap. An external magnetic field is used as a control ensuring the existence of plasma column away from the vacuum container wall.

We consider the Vlasov-Poisson system of equations in infinite cylinder with nonlocal boundary conditions for potential of self-consistent electric field and initial conditions for density distribution functions. It is proved existence and uniqueness of classical solution with support inside cylinder for sufficiently small initial density distribution functions and sufficiently large homogeneous field directed along the axis of cylinder. This statement generalizes the results of [1].

This research was carried out with the support of RFBR (grant N 12-01-00524).

References

1. A.L. Skubachevskii, Vlasov-Poisson Equations for a Two-Component Plasma in a Homogeneous Magnetic Field, *Uspekhi Mat.Nauk*, 69 (2014), 107-148; English transl. in *Russian Math. Surveys*, 69 (2014).

Reaction-diffusion systems with hysteresis

Pavel Gurevich
gurevich@math.fu-berlin.de

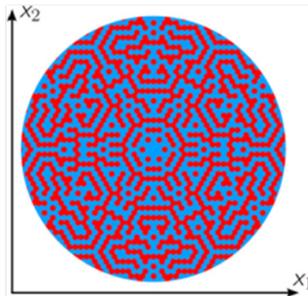
Free University of Berlin

In biological and population models, diffusive and nondiffusive substances often interact with each other according to hysteresis law [1]. In the lecture, we discuss a corresponding prototype mathematical model. This will be a reaction-diffusion equation with a hysteretic nonlinearity. In the first part of the lecture, we will show how this nonlinearity gives rise to slow-fast dynamics and what the limitations for the initial data are [2].

What happens beyond those limitations is the subject of the second part of our lecture. We will consider a spatially discrete analogue of the above continuous system. This will have much to do with dynamics on lattices, networks, and graphs. We will demonstrate a new self-organization phenomenon which leads to pattern formation (see the figure where two different colors represent two different hysteresis states at a fixed time moment) and present the main ingredients which can explain it.

This is a joint work with Sergey Tikhomirov. The research was supported by the DFG project SFB 910 and by DAAD through the G-RISC project.

2D domain
(triangular lattice)



References

1. F.C. Hoppensteadt, W. Jäger // Lecture Notes in Biomathematics, 38, p. 68-81 (1980).
2. P. Gurevich, S. Tikhomirov // Mathematica Bohemica, 139, No. 2, p. 239-257 (2014).

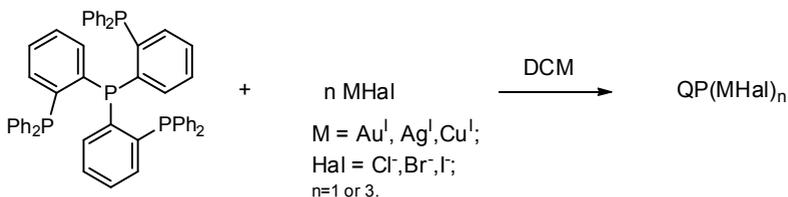
A. Chemistry

Solid-state luminescence of Au(I), Ag(I) and Cu(I) complexes with tetradentate phosphine ligand

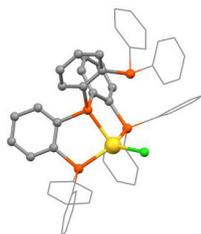
Beliaev Andrei
andreibelyaev07@gmail.com

Scientific supervisor: Dr. Krupenya D.V., Department of General and Inorganic Chemistry, Institute of Chemistry, Saint-Petersburg State University

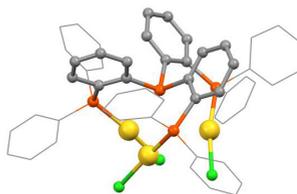
Reactions of tetradentate tris[(2-diphenylphosphino)phenyl]-phosphine (QP) with halides of coinage metals yield a new series of complexes with general formula QP(MHal)_n.



The compounds obtained were characterized by ¹H and ³¹P NMR spectroscopy and ESI-MS measurements. The solid state structures of some complexes have been elucidated by X-ray crystallography.



QPAuCl



QP(AuCl)₃.

All complexes display intensive luminescence in the solid state at room temperature, but don't emissive in solutions. A large Stokes shift and microsecond excited state lifetimes indicate triplet nature of the luminescence.

The work was carried out using scientific equipment of the Center of Shared Usage "The analytical center of nano- and biotechnologies of SPbSPU" with financial support of the Ministry of Education and Science of the Russian Federation and Research Park of St. Petersburg State University: X-ray Diffraction Center; Center for Magnetic Resonance; Center for Optical and Laser Materials Research; Center for Chemical Analysis and Materials Research. Financial support from Saint-Petersburg State University research grant 0.37.169.2014 and Russian Foundation for Basic Research (grant 14-03-00970) are gratefully acknowledged.

Synthesis of B-homo analogues of steroid estrogens

Drozdov Andrey
mail.to.drozdovl@gmail.com

Scientific supervisor: Prof. Dr. Shavva A.G., Department of Natural Compounds Chemistry, Faculty of Chemistry, Saint-Petersburg State University

Estrogens play an important role in many biological processes. Because of the regulatory function estrogens play an important role in cancer development. Up to 95% of human breast cancers, at the origin, are hormone-dependent. By combination of different modifications it is possible to alter biological activity of the estrogen analogue to use it as drug [1]. Most important modifications are to reduce hormonal activity of the analogue, to reduce toxicity of its metabolites and to introduce some new biological activity, e.g. ability to inhibit estrone sulfatase [2].

B-homo analogues of steroid estrogens (Fig. 1) are representing interesting class of estrogens. Conformational mobility of 7-member B ring reduces hormonal activity of these analogues and may prevent formation of cancerogenic metabolites. Further modifications may make them potential anticancer agents.

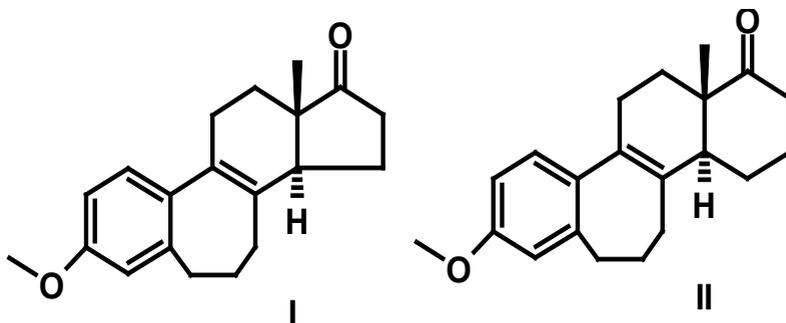


Fig. 1. B-homo analogues of steroid estrogens.

References

1. R. Maltais, M.R. Tremblay, L.C. Ciobanu, D. Poirier // *J. Comb. Chem.*, v. 6, № 3, p. 443-456 (2004).
2. H. Lawrence, N. Vicker, G.M. Allan, A. Smith, M.F. Mahon, H.J. Tutill, A. Purohit, M.J. Reed, B.V.L. Potter // *J. Med. Chem.*, 48, 2759 (2005).

Prospects of biodiesel production using coupled processes

Golikova Alexandra, Toikka Maria
al.golikova@gmail.com
masha-toikka@yandex.ru

Scientific supervisor: Prof. Dr. Toikka A.M., Department of Chemical Thermodynamics and Kinetics, Institute of Chemistry, Saint-Petersburg State University

At present time the number of cars is almost equal to the number of people in the world. And this is just one sphere of industry, which use oil and gas. The amount of harmful emission into the atmosphere can be called critical already for a long time. **Scientists all over the world are looking for renewable and environment friendly sources of energy.**

One of these fuels is biodiesel. This fuel is obtained using reaction of transesterification of fatty acid and methanol. Fatty acids contain in a variety of vegetable oils. This paper discusses the alternative process of production of diesel fuel. There are data on conversion of rapeseed oil into esters. It consists of addition of supercritical fluids (ether: ethyl acetate, methyl acetate, etc.) at the temperature of 350 °C and pressure up to 17.8 MPa without using a catalyst with extremely high yield of the final product [1].

This study is directed to a detailed physico-chemical study of coupled processes in the technology of biofuels. The chemical equilibrium of quaternary system acetic acid - ethanol - ethyl acetate - water was studied at 40°C. The research was performed by two different methods: the classical method of gas chromatography and relatively new one for this theme – by nuclear magnetic resonance method.

This research was supported by Committee on Science and Higher Education of St. Petersburg for young scientists, young PhD, industry and academic institutions located in the territory of St. Petersburg (2013, Toikka Maria).

References

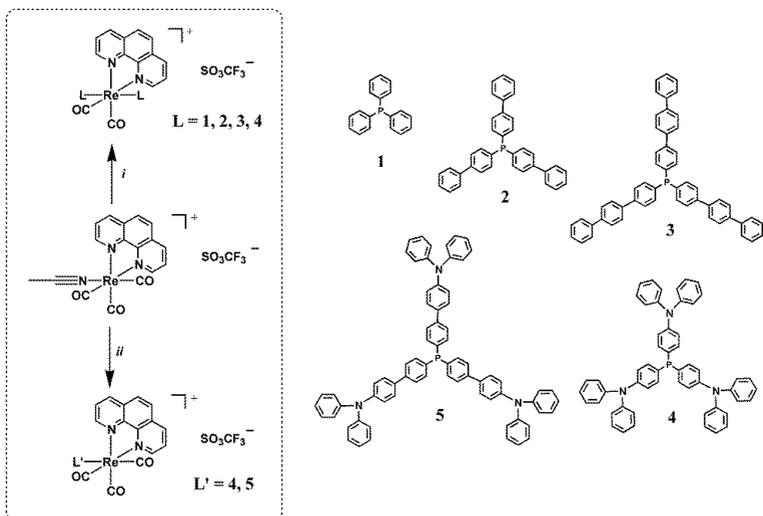
1. Goembira F., Matsuura K., Saka S. Biodiesel production from rapeseed oil by various supercritical carboxylate esters. *Fuel*. 2012.

Rhenium (I) diimine complexes with extended chromophoric phosphines

Kisel Kristina
kristinakisel@yandex.ru

Scientific supervisors: Koshevoy I.O., Grachova E.V., Institute of Chemistry, Saint-Petersburg State University

Rhenium(I) diimine complexes represent a versatile class of organometallic luminophores. A wide range of these compounds was prepared and investigated over the decades particularly due to their rich photophysical characteristics as well as attractive coordination chemistry. Here in we report an overview of six novel synthesized complexes of rhenium(I) which have been prepared according to the following scheme:



Reaction conditions: i – autoclave, 180 °C, 30 bar, toluene, 16 hours, under nitrogen; ii – autoclave, 130 °C, 30 bar, toluene, 16 hours, under nitrogen.

Complexes [Re(CO)₃(phen)(L)](SO₃CF₃) and [Re(CO)₂(phen)(L)₂](SO₃CF₃) were characterized by ¹H and ³¹P NMR spectroscopy, IR spectroscopy, mass-spectrometry (in a solution), and by X-ray diffraction analysis (in solid state).

It has been found that the complexes **1–3** are emissive in the yellow region of the spectrum, and **4** in the orange region of the spectrum, while the compound **5** shows luminescence in the green region of the spectrum upon photoexcitation $\lambda_{ex} = 410$ nm.

The authors greatly appreciate the financial support of St. Petersburg State University research grants 0.37.169.2014, 12.42.1263.2014 and Russian Foundation for Basic Research grant 13-04-40342.

The activation mechanism of gold for oxidation reactions

Klyushin Alexander
klyushin@fhi-berlin.mpg.de

Scientific supervisors: Prof. Dr. Schlögl R., Department of Inorganic Chemistry, Fritz-Haber-Institut der Max-Planck-Gesellschaft; Prof. Dr. Vinogradov A.S., Department of Physics, Saint-Petersburg State University

The discovery, that nanoscopic gold particles supported on metal oxides are active for low-temperature CO oxidation, has inspired a considerable amount of research directed toward understanding the basis for the activity of Au catalysts [1]. Different factors such as quantum size effects, low coordinated atoms, surface ions and the support interaction [2] have been proposed to effect on Au activation. Here we report the systematical study of the activation mechanism of Au in CO oxidation reaction.

All measurements were performed in the near ambient pressure X-ray photoelectron spectroscopy (NAP-XPS) endstation at the ISSS beamline at HZB/BESSY II (Berlin, Germany). Gold containing samples (Au foil, Au nanoparticles (NPs) supported on carbon and transition metal oxides) were characterized using *in-situ* XPS, SEM and TEM techniques. CO and O₂/O₃ was introduced to the chamber at different ratio keeping the pressure of 0.3 mbar and the temperature of 100 °C.

Our *in situ* measurements show that the activation of extended Au surfaces by O₃ treatment is accompanied by the formation of a surface oxide phase, however this phase is metastable and decomposes both in vacuum and under reaction conditions [3]. Consequently, Au-oxide does not directly participate in the CO oxidation on Au catalysts. Au NPs on oxygen-free support do not show any catalytic activity regardless of the NPs' size and the type of the support, therefore the size reduction and/or the oxidation is not enough to activate Au.

The formation of two Au species (Au⁰ and Au^{δ+}) on the surface of active Au/TiO₂ and Au/Fe₂O₃ samples was found. TEM images indicate the formation of support layer on top of Au particles. All these results suggest Au activation via Strong Metal Support Interaction, assuming strong influence of the support on the electronic structure of the gold through charge transfer and stabilization of low-coordinated Au atoms.

References

1. B.K. Min, C.M. Friend // Chem. Rev., v. 107, № 6, 2709-2724 (2007).
2. R. Meyer, C. Lemire, Sh.K. Shaikhutdinov, H.-J. Freund // Gold Bulletin, v. 37, № 1-2, 72-124 (2004).
3. A.Yu. Klyushin, T.C.R. Rocha, M. Hävecker, A. Knop-Gericke, R. Schlögl // PCCP, v. 16, № 17, 7881-7886 (2014).

Synthesis of 5-amino-1,2,4-oxadiazoles via Zn^{II}-catalyzed reaction of amidoximes and cyanamides

Kulish Kirill
kulish_kirill_92@mail.ru

Scientific supervisor: Prof. Dr. Bokach N.A., Department of Physical Organic Chemistry, Institute of Chemistry, Saint-Petersburg State University

1,2,4-Oxadiazoles represent an important class of five-membered heterocycles, and their versatile chemistry has been repeatedly reviewed over the years. These species are currently evaluated in numerous therapeutic areas, as they behave as anti-inflammatory agents, receptors agonists and antagonists, hypocholesterolemic agents, and antiviral agents. Very recently, a series of 3-aromatic-5-amino-1,2,4-oxadiazoles were proved to be potent therapeutic agents for prostate cancer [1]. Among numerous ways of 5-amino-1,2,4-oxadiazoles generations we have chosen method which consist of amidoxime and cyanamide coupling in presence of Zn^{II}. We found that 5-amino-1,2,4-oxadiazoles can be prepared by this method with higher yields and with milder conditions compared to known literature data. The heterocyclization (Fig. 1, B) is not affected by the presence of the metal and only the first step required Zn^{II} (Fig. 1, A), therefore the generation of the oxadiazoles could be conducted as Zn^{II}-catalyzed rather than Zn^{II}-mediated reaction [2]. Thus, our work demonstrate rapid formation of 5-amino-1,2,4-oxadiazoles from amidoximes and cyanamides with good yields.

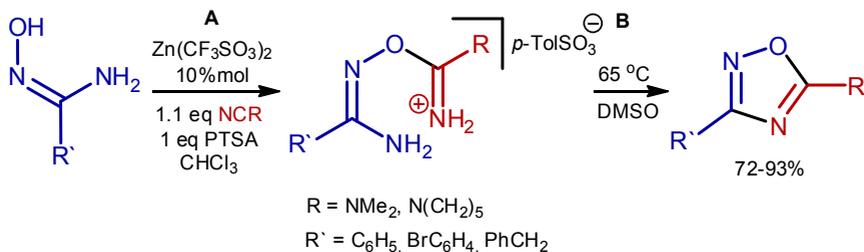


Fig. 1. Catalytic approach to 5-amino-1,2,4-oxadiazoles.

This work was supported by the Russian Science Foundation (grant 14-13-00060).

References

1. A. Pace, S. Buscemi, and N. Vivona // *Org. Prep. Proced. Int.*, v. 37, pp. 447-506 (2005).
2. D.S. Bolotin, K.I. Kulish, N.A. Bokach, V.Yu. Kukushkin // *Inorg. Chem.*, 53, 10312–10324 (2014).

Quantum-chemical simulation of the interaction of phenols with potassium carbonate in the presence of hematite

Lyutkin Andrew
andrewstudent@rambler.ru

Scientific supervisor: Dr. Orlov V.Yu., Department of Organic and Biological Chemistry, Demidov Yaroslavl State University

We have studied the effect of additives iron oxide (III) for the formation of bi-phenyl ethers in the reaction p-nitrochlorinebenzene with phenoxide anions formed in situ (by reacting the phenol with potassium carbonate). Experiments carried out with the addition of various samples of hematite in the reaction system showed that the introduction of the solid component accelerates passing of the process to varying degrees. The greatest influence on the studied reaction has iron oxide (III), obtained from ferrous sulfate. To evaluate the features of flow mechanism of the studied process was used quantum-chemical modeling of reaction systems on the basis of PM7. In order to study the structure of the reaction center in the presence of hematite was used to simulate the interaction of phenol with iron oxide (III) and potassium carbonate. At the same time geometry optimization and study the dependence of the energy system of bond length O21-H27 from the initial value 3 Å to 7 Å in steps of 1 Å are carried out.



.Fig. 1 Quantum-chemical modeling of the interaction of phenol with potassium carbonate (a) and iron oxide (III) (b)

Results showed that most likely is the formation of iron oxide (III) - phenol and its following reaction with potassium carbonate. This leads to accelerated formation of the phenoxide anion.

Photochemistry of Copper(II) Chlorocomplexes in Acetonitrile Studied by Means of Femtosecond Transient Absorption Spectroscopy

Mereshchenko Andrey, Pavel Olshin
andrey@chem.spbu.ru

Scientific supervisor: Dr. Tver'yanovich Yu.S., Institute of Chemistry, Saint-Petersburg State University

Photochemistry of three copper(II) chlorocomplexes in acetonitrile solution, CuCl^+ , CuCl_3^- , and CuCl_4^{2-} , was studied by the combination of the steady-state photolysis and time-resolved ultrafast spectroscopy methods enabling us to reveal the main relaxation pathways of the initially excited Ligand-to-Metal Charge Transfer (LMCT) state. The major fraction of the LMCT-excited copper(II) chlorocomplexes undergoes internal conversion to the vibrationally relaxed ground state parent complex through the vibrationally hot ground and LF excited states. Minor fraction of the LMCT excited $[\text{Cu}^{\text{II}}\text{Cl}_{n-1}]^{2-n}$ complexes dissociates forming either ionic products without photoreduction of copper(II) ($[\text{Cu}^{\text{II}}\text{Cl}_{n-1}]^{3-n} + \text{Cl}^-$) or radical products with photoreduction of copper(II) to copper(I) ($[\text{Cu}^{\text{I}}\text{Cl}_{n-1}]^{2-n} + \text{Cl}^-$). The ionic dissociation occurs from the different LMCT states, whereas radical dissociation mainly originates from the lowest energy LMCT state. The products of ionic dissociation recombine back to the parent complex due to high lability of the copper(II) complexes. The products of radical dissociation partially recombine back to the parent complex. However, a portion of radical dissociation products undergoes further reactions, e.g. reaction with the solvent molecules, resulting in long-lived photoreduction products including copper(I) complexes. The quantum yield of the photolysis, copper(II)-to-copper(I) photoreduction, is defined by the initial ultrafast steps and is not affected by the presence of the oxygen. Thus, the CuCl^+ complex has largest photoreduction quantum yield, about 5%, which corresponds to the maximum yield of the radical dissociation products at 1 ns, about 20%. The CuCl_3^- complex has the intermediate photoreduction quantum yield, about 1.5 %, corresponding to the intermediate yield of the radical dissociation products at 1 ns, about 2%. The CuCl_4^{2-} complex is found to be photostable, which is in agreement with ultrafast data, where only one dissociation channel, ionic dissociation, was detected.

Acknowledgments

A.S.M acknowledges the Saint-Petersburg State University for the financial support (postdoctoral fellowship No. 12.50.1562.2013). Steady-state photolysis measurements were performed at the Center for optical and laser materials research of Saint-Petersburg State University. Measurements of the individual absorption spectra of copper(II) chlorocomplexes and transient absorption measurements were performed at the Center for Photochemical Sciences of Bowling Green State University. This work was supported by RFBR (Grant 14-03-01003).

Structural and optical properties of glasses $A_2O-P_2O_5-Nb_2O_5$ (A=Li, Na, K)

Olshin Pavel, Vasil'eva Anna, Kireev Alexey, Manshina Alina,
Sokolov Ivan
pavel_olshin@bk.ru

Scientific supervisor: Dr. Povolotskiy A.A., Department of Laser Chemistry and Laser Materials, Institute of Chemistry, Saint-Petersburg State University

The aim of this work is an investigation of the optical and structural properties of alkali-phosphorus glasses containing niobium oxide (Li_2O (Na_2O , K_2O) – P_2O_5 – Nb_2O_5).

Structural properties were studied by Raman and IR spectroscopy. Raman spectra were received using the spectrometer Bruker Senterra, excitation wavelength was 532 nm. IR spectra were measured by Nicolet 8700 (Thermo Scientific).

Optical properties – refractive indexes and absorption spectra were studied. Refractive indexes were measured by refractometer IRF-23, absorption spectra were obtained by spectrophotometer Lambda 1050 (Perkin Elmer).

The Raman and IR spectra show redistribution of peak intensities occurring in glasses with composition changes. Decreasing of atomic weight of alkali metal leads to peaks shift in low-frequency region. The dependence of the peak position on glass composition has been demonstrated. Refractive index increases as niobium oxide concentration grows.

Crystallization ability for some glasses was considered. Glasses were heated up to glass transition temperature. The temperature was held for two hours. The temperature was raised to 650 °C and was held for two hours. After annealing glasses were cooled with the furnace. Crystalline nucleus in considered glasses were found after annealing by Raman spectroscopy.

Acknowledgements

Raman, IR, absorption spectra were obtained at the Center for Optical and Laser Materials Research of Saint-Petersburg State University.

Supported by the Ministry of Education and Science of the Russian Federation (№ 14.576.21.003).

A new method for the isolation and concentration of the herbicide glyphosate and its major metabolite aminomethylphosphonic acid

Shreyner Ekaterina
shreyner.ekaterina@gmail.com

Scientific supervisors: Podolskya E.P., Alexandrova M.L. Institute of Toxicology of the Federal Medical and Biological Agency, Saint-Petersburg

Because of the intensive use of pesticides in modern agricultural industry in the last decades of their content in the objects of environmental increased significantly. In this regard, the development of new highly specific and selective analytical methods for the monitoring and measuring the level of pesticides in the environment is a promising task.

The glyphosate and its metabolite aminomethylphosphonic acid (AMPA) has been chosen as an object, because these pesticides are widespread herbicide and have a high degree of toxicity. Furthermore, in recent years, many researchers suggest that glyphosate can affect the health of animals and humans [1].

In connection with the specific physical and chemical properties of glyphosate and AMPA (low volatility, lack of chromophore groups, low solubility in organic solvents) determination of these compounds in samples of different nature is a laborious, complicated and expensive process.

We have proposed an entirely new method of extraction and concentration these pesticides from an aqueous solution without a pretreatment of the sample without using any derivatizing agent. This method includes conducting metal-affinity chromatography using a newly developed sorbent based on nanoregularity structures (NRS) [2], copper (II) and nickel (II) oxide followed by eluting components using different solvents (ammonia and piperidine). Quantitative analysis was performed by AES with ICP. The results are shown in Fig. 1.

Based on these data, we conclude that isolation of glyphosate and AMPA from aqueous solutions using NRS-based nickel (II) and copper (II) followed by elution of the compounds is possible.

References

1. José L. Tadeo. Analysis of Pesticides in Food and Environmental Samples.- CRC Press, 2008. -359 p.
2. A.A. Selyutin et al. // Scientific instrumentation, 2013, v. 23, № 1, pp. 115–122.

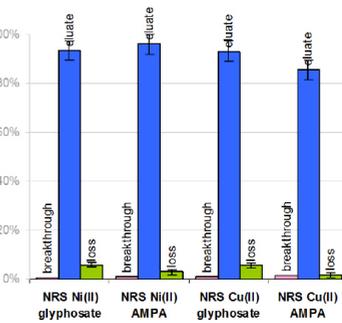


Fig. 1. Results of metal-affinity chromatography NRS Cu (II) and NRS Ni (II) for glyphosate and aminomethylphosphonic acid.

Influence of industrial pollutions on a chemical composition and morphology of some medicinal plants

Solovyeva Natalia, D.M. Toropova, Y.G. Oleneva, A.I. Ivanova,
S.D. Khizhnyak, P.M. Pakhomov
natulka511u@mail.ru

Scientific supervisor: Prof. Dr. Pakhomov P.M., Department of Physical Chemistry, Chemistry Faculty, Tver State University

One of plants features is the ability to accumulate different substances from the environment, including toxic. Moreover, under adverse conditions of the environment the content of phenolic compounds can increase in plants. Phenolic compounds play a role of protective barrier on a way of mechanical, chemical, thermal factors of the environment, and also pathogenic influences. So, actual task is the studying of chemical composition changes of medicinal plants as a consequence the influence of anthropogenic factors. It's important to estimate the quality of medicinal raw materials from one hand and the degree of environmental pollution from the other hand. The aim of the research is the evaluation of the industrial pollution impact on the chemical composition and morphology of yarrow (*Achillea millefolium*), plantain (*Plantago major*), dandelion (*Taraxacum officinale*) using methods of FTIR and UV spectroscopy, AAS and SEM. Different kinds of the medicinal herbs for the study are collected from the same industrial areas of the town Tver (Thermal Power Stations, Railcar plant, The Paint Factory, The Printing Plant) with different environmental stress. Finished pharmaceutical forms of yarrow and plantain of the firm "Health" have been chosen as a control sample.

The results showed that the chemical composition of the analyzed medicinal plants susceptible to the influence of anthropogenic factor. In the IR spectra of samples collected from different sites there are differences for the following characteristic absorption bands (intensity and position of the maximum): $\sim 1740\text{--}1734\text{ cm}^{-1}$ ($\nu_{\text{C=O}}$), $\sim 1656\text{--}1620\text{ cm}^{-1}$ ($\nu_{\text{C=C}}$), $\sim 1541\text{--}1516\text{ cm}^{-1}$ (Amide II), $\sim 1107\text{--}1024\text{ cm}^{-1}$ ($\nu_{\text{C=O}}$, $\nu_{\text{C=C}}$, $\nu_{\text{C-O-C}}$). Besides, there are differences in UV absorption spectra of the alcoholic extracts in the region of 200–500 nm, which indicate the change of the composition and concentration of phenolic compounds in the samples depending on the sites of gathering. It is found out that content of some heavy metals (Fe, Zn, Mn, Cu, Cr, Pb, Co, Cd) detected in the samples by means of AAS is changed in a wide range in dependence on the kind of the herbs and on the site of collection. Morphological changes of the leaves have been studied by the help of the SEM and showed big difference in the structure. Thus, it has been proved by various techniques (FTIR, UV spectroscopy, AAS and SEM) that the chemical composition and the leaves structure of the medicinal herbs depend on the environment condition that should be considered in preparation of the finished pharmaceutical forms.

B. Geo- and Astrophysics

Interference seismic waves

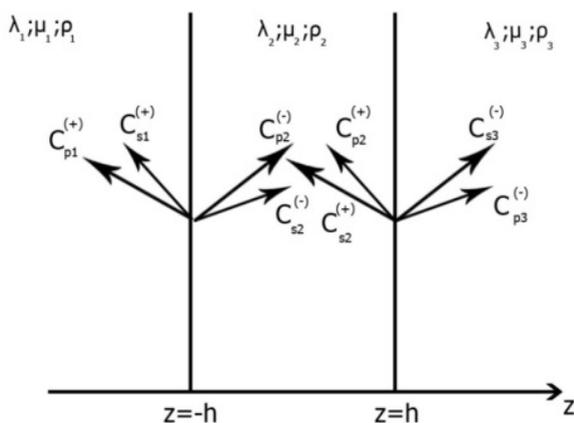
Bazulin Maksim
maxandr93@mail.ru

Scientific supervisor: Prof. Dr. Kashtan B.M., Department of Earth's Physics, Faculty of Physics, Saint-Petersburg State University.

There are a lot of boundaries between rocks with different elastic properties in the real geological sections. Therefore, research of wave fields in layered media is a particular interest for seismic prospecting [1].

First of all, we construct a model of the geological environment, than we search for a solution of the equation of motion of an elastic isotropic medium. After that, we form the dispersion equation and search for its roots. Than we can analyze dependence of the wave velocity of its frequency and thickness of the layer [2].

For the beginning, we search solutions of dispersion equation for medium with one interface (e.g. contact of two different elastic media). Than we sophisticate a model of the geological environment, and solve corresponding dispersion relation [2]. In the end, we analyze problem of elastic layer between two elastic media with slide contact.



References

1. Viktorov I.A. Physical basis of the application of ultrasonic waves Rayleigh and Lamb M.: Science (1966).
2. Brekhovskikh L.M. Waves in layered media. - M.: Science (1973).

Analysis of the observations of CO₂ concentrations in the ambient air at the Peterhof station

Foka Stefani
Stesy16@mail.ru

Scientific supervisor: Dr. Makarova M., Department of Atmospheric Physics, Faculty of Physics, Saint-Petersburg State University

Carbon dioxide (CO₂) is an important long-lived greenhouse gas in the Earth's atmosphere. Since pre-industrial period CO₂ concentrations in the atmosphere have risen by over 30%. Ground-based observational networks, aircraft campaigns, satellite experiments together with the powerful tools of atmospheric modeling are focused on the investigations of past, present and future of CO₂ in the atmosphere.

The Peterhof station (SPbU) of atmospheric monitoring is located in the building of Institute of Physics, 35 km to the west from the city center. High accuracy measurements of CO₂ concentrations in the ambient air are being carried out by Los Gatos Research Greenhouse Gas Analyzer 24r-EP from 2013.

The main targets of this study are as follows:

- to estimate temporal variations of CO₂ concentration for the Peterhof station;
- to compare our results with independent measurements and modeling results;
- to indicate reasons which could be responsible for the variations of CO₂.

Analysis of CO₂ concentrations for 2013 revealed pronounced annual cycle of CO₂ with the amplitude of 2.5% (from the average CO₂ level of 403 ppm). The range of CO₂ monthly means (391-408 ppm) for Peterhof agrees with the WMO (World Meteorological Organization) reference levels of CO₂ (360 - 450 ppm) for the unpolluted air. It was also shown that CO₂ concentrations at the Peterhof station have diurnal variations with amplitude that varies from 1% in December up to 6% in June. The analysis of our CO₂ data in comparison with CO₂ measurements at two high latitude stations Teriberka and Tiksi demonstrates that both, annual and diurnal cycles of CO₂ are controlled by following main factors: geographical location, climate, atmospheric transport (intensity of vertical transport in the troposphere), natural (respiration processes) and anthropogenic (fossil fuel combustion) sources of CO₂, and CO₂ sinks (photosynthesis process).

Analysis of CO₂ variations for the February of 2013 together with the results of HYSPLIT model and meteorological data shows that the highest values of CO₂ (up to 470 ppm) were registered at the Peterhof station for calm conditions which were enhanced by the presence of temperature inversions (the case of the intensive accumulation of anthropogenic emissions in the boundary layer).

Acknowledgements

Investigations were supported by Russian Science Foundation (grant №14-17-00096). Author thanks Geomodel Research Center (SPbU) for the providing of observational facilities.

Gydra - GPU-based code for astrophysical SPH simulations

Korsunov Igor
elquendi@yandex.ru

Scientific supervisor: Prof. Dr. Khoitygin A.F., Chair of Astronomy, Mathematics and Mechanics Faculty, Saint-Petersburg State University

A smooth particle hydrodynamics (SPH) is a well-known computational method used as a tool for modelling many astrophysical processes from cosmological structure formation to stellar winds and formation of stars.

There are several state-of-the-art SPH codes for astrophysics (e.g., Gadget2 and Fi). Many of these codes are parallel and/or distributed, but none of the major SPH solvers use GPU though the method itself should be well suited for GPU model of computation.

We present Gydra - proof of concept SPH solver for astrophysics, implemented in C++ and CUDA with the help of the Thrust library. It is intended to use GPU implementation of octrees both for finding nearest neighbour particles and for calculating gas self-gravity via Barnes-Hut algorithm.

Spectral properties of the X-ray binary GX339-4

Kosenkov Ilia, Zabelina Natalia
ilia.kosenkov.at.gm@gmail.com

Scientific supervisor: Prof. Dr. Poutanen Ju., Director of Tuorla Observatory, Finland

The nature of the X-ray binary GX339-4 was investigated. O/IR observations of GX339-4 were obtained from Buxton M. [1]. The source was monitored by SMARTS 1:3m telescope on a near-daily basis in 4 filters: optical (V) and infrared (I; J; H). X-ray observations were taken from ASM RXTE project. The shapes of spectra of this black hole binary obtained during 2002-2010 in O/IR and X-ray show that there are two possible states of the source. The radiation is emitted by the accretion disk of black hole and outbursts should correspond to some internal processes of the disk. According to standard model, emission is originating in irradiated disk [2]. Thus, the spectra of such component are expected to be close to black body's.

There is no agreement between the values of extinction to the source [3]. An independent estimates of A_V parameter were made. Extinction in other bands were calculated using models suggested in [4] and [5]. Photometric zero-point fluxes were taken from [6]. Some observations provide an opportunity to separate black body component from others right before or after an outburst. Extrapolated BB spectrum can then be subtracted to reveal the second non-thermal component. This enables to study both BB and non-BB units separately. Each obtained measurement of flux from the source can be used to estimate size of radiating disk in distance to the object units. Using some calculated in advance values of distance to GX339-4 [7] we acquired the size of the accretion system surrounding the black hole. These measurements agree with upper limits set by the size of Roche lobe for BH and in influence caused by tidal forces.

The evolution of the source and its states was traced by analyzing light curves obtained from observations in O/IR. The most powerful outbursts discovered in these bands are often followed by similar outbursts in X-ray.

We performed a complex analysis of observational data in O/IR and X-ray of the GX339-4. We studied spectral properties during different outbursts in a 8-year period. A two-component model of the source was suggested. Spectrum of one component is close to black body's. Value of the effective radius of the accretion disk was estimated.

References

1. Buxton M.M., Bailyn C.D., Holly C.L. et al. // 2012, ApJ, 143, 130.
2. Poutanen J., Veledina A., 2014, MNRAS.
3. Homan J., Buxton M., Marko S. et al. // 2005, ApJ, 624, 295.
4. Cardelli J.A., Clayton G.C., Mathis J.S. // 1989, ApJ, 345, 245.
5. O'Donnell J.E. // 1994, ApJ, 422, 158.
6. Bessell M.S., Castelli F., Plez B. // 1998, A & A, 333, 231.
7. Kalemci E., Din cer T., Tomsick J.A., Buxton M.M., Bailyn C.D., Chun Y.Y. // 2013, ApJ, 779/2, 95.

Spectral characteristics of sources located above the neutral line of the photospheric magnetic field and their connection with flares

Kurochkin Evgenii
79046155404@yandex.ru

Scientific supervisor: Prof. Dr. Yasnov L.V., Department of Radio Physics, Faculty of Physics, Saint-Petersburg State University

In this research we analyse multiwave spectral and polarized characteristics of the peculiar radio sources in the active regions located above the area with the neutral line of the photospheric magnetic field. The analysis was being held in a wide range of waves while making multi-azimuth observations (up to 32 observations per day) and correlating with eruptive processes in the active region (radio pulses, flares in X-rays). The evolution of the radio spectra is noticed due to the uprise of a new magnetic flux. Some possible interpretation of the mechanism of occurrence of a new peculiar source and an acceptable model consistent with the observed data are produced.

Russian aeromagnetic exploration and complex airborne geophysics at the start of a new phase – use of unmanned aviation vehicles

Kuznetsova Anna
geolraz@geolraz.com

***Scientific supervisors: Dr. Tsirel V.S., “Geologorazvedka” company;
Korotkov V.V., “VIMS” company***

History. 1995, the first ever published suggestion of using unmanned aviation vehicles (UAV) in aerogeophysics by VIRG – Rudgeophysica, Saint-Petersburg [1]. Heavily limited capabilities of UAV at the time.

Main tasks. Application of aerogeophysics to exploration of the nearsurface stratum; larger scale surveys to enhance the role of geophysics at the final stage of geological exploration. Additional possibilities for ecological or engineering research.

Topicality. Sharp rise in the rent of usual piloted aircraft resulting in an important rise of airborne surveys price; demand for a better suitability of air vehicles; problem of personnel safety; necessity for research in difficult territories.

General list on the basis of UAV: detailed prospecting of ore-bearing fields; delineation of ore controls and structures; analysis for local deposits of economic hard minerals; exploration for fresh water; exploration of oil and gas structures and salt domes etc.

Analysis of domestic UAVs available in Russia – choice of those most suitable for bearing both complex or monomethod aeromagnetic equipment. Statement of demands for the possible use of UAVs. Hence – necessity for the combined efforts of both UAV and geophysical equipment designers.

Information on airborne geophysical surveys with the use of UAVs abroad. Absence of international rules concerning UAVs flights. Available types of foreign made UAVs. 2012-2013 aeromagnetic and airborne electromagnetic surveys for mapping geothermal sources.

Summary. Importance of starting scientific research and experimental constructor activities for creating a new type of aerogeophysical surveys allowing for solving a large spectrum of geological, ecological and engineering problems.

The author would like to express her deep gratitude to supervisors of the project Vadim Solomonovich Tsirel, Doctor of Geophysics, Head of the Department of Science Methodology of the “Geologorazvedka” company and Vladimir Victorovich Korotkov, Deputy Director General of the “VIMS” company for the fruitful discussions and valuable advice.

References

1. Vorobyev V.P., Glagolev V.A., Kirsanov V.N., Nahabtsev A.S., Filimonov V.V., Tsirel V.S. Prospects for the usage of airborne geophysical method for detailed geophysical works. *Geofizicheskaya apparatura [Geophysical instrument]*. Leningrad: Rudgeopfizika., no. 100 (1995), 117-126.

Photometry and polarimetry of supernovae performed on telescopes LX200 and AZT-8

Mokrushina Anna
hobbitenka1608@rambler.ru

Scientific supervisor: Head of the Laboratory Arkharov A.A., Laboratory of Physics of Stars and Galaxies, The Central (Pulkovo) Astronomical Observatory of the Russian Academy of Sciences

Supernovae are an important subject of research, because in the process of thermonuclear synthesis they form the diversity of the chemical elements that make up the rest of the objects in the universe. Their study helps to understand better the evolution of matter in the universe. The relevance of the study of these objects supports the recent discovery of the accelerated expansion of the universe, made as a result of the study of supernovae.

Observations, processing and analysis of the data obtained were made of supernova 2013ej (type IIP) and 2014J (type Ia). As a result of observations there were made plots the light curves, the analysis of which allowed to calculate the following physical parameters: bolometric luminosity [1], bolometric correction [1], the mass ejected in the explosion of a nickel [1], the explosion energy, the mass of the ejected shell radius of the star - the progenitor, the temperature distribution and the radius of the photosphere, depending on the time, estimate of the distance to the supernova [2]. Both supernovae have shown a fairly high degree of polarization, which may indicate a large asymmetry of the explosion [3].

References

1. K. Maguire, E.Di Carlo, S. J. Smartt, A. Pastorello, A.A. Arkharov, V.M. Larionov, S. Valenti // Notices of the Royal Astronomical Society, 2:981-1004, (2010).
2. Mario Hamuy // The Astrophysical Journal, 2:63-65, (2002).
3. D. Andrew Howell, Peter Hoflich, Lifan Wang, J. Craig Wheeler // The Astrophysical Journal, v.556, 1:302-321, (2001).

Correlation of radial fluctuations in deep galaxy redshift surveys

Shirokov Stanislav
lakronous@mail.ru

Scientific supervisor: Dr. Baryshev Yu.V., Department of Astrophysics, Faculty of Mathematics & Mechanics, Saint Petersburg State University

One of the most important problems in modern observational cosmology is to determine the maximal size of large-scale inhomogeneities in distribution of galaxies in the Universe. For this purpose a comparison of radial fluctuations in two deep galaxy redshift surveys (COSMOS and UVISTA) is considered.

Correlation analysis was performed for photometric redshift catalogs in the optical COSMOS [1] and in the infrared range UltraVISTA [2]. The method first proposed in [3] of estimation of sizes and amplitudes of radial fluctuations for different redshift bins was used. The Pearson correlation coefficient between two independent samples of fluctuations has the value $R = 0.69 \pm 0.16$ for redshift interval $0.1 < z < 3.5$. This correlation observed between independent surveys of different research groups confirms the existence of super-large galaxy structures with sizes up to 1000 Mpc/h.

The resulting fluctuation picture of the visible matter distribution shows that linear dimension of inhomogeneities essentially exceeds LCDM model predictions [4] and that observed fluctuation amplitude at factor 2-3 larger than predicted by biasing model [5].

References

1. Ilbert O., Capak P. et al. // *Astrophys. J.*, 690, 1236 (2009).
2. Muzzin A. et al. // *Astrophys. J. Suppl.*, 206, 19 (2013).
3. Nabokov N.V., Baryshev Yu.V. // *Astrophysics*, 53, 101 (2010).
4. Sylos Labini F., Vasilyev N.L. // *Astron. Astrophys.*, 477, 381 (2008).
5. Moster B. et al. // *Astrophys. J.*, 731, 113 (2011).

The Spatial Distribution of Galaxies in 2MRS and SDSS Catalogs

Tekhanovich Daniil
foobat@yandex.ru

Scientific supervisor: Dr. Baryshev Yu.V., Faculty of Mathematics and Mechanics, Saint-Petersburg State University

A problem of studying large scale structure of the Universe by statistical analysis of galaxy catalogs was considered. We choose two catalogs of spectroscopic galaxy redshifts which covers different areas on the sky and consist of different types of galaxy since selection was made in different photometric bands. From each catalog we select volume limited samples and test their completeness and absence of selection effects by new method of tiny cylinders [1]. Correlation properties in selected samples was studied by counts in spheres [2]. It was shown that galaxies in 2MRS and SDSS catalogs tends to show same behavior and are characterized by power-law correlations with exponent $\gamma=0.9$ up to 20 Mpc/h and transition to $\gamma=0.3$ in the range 20-100 Mpc/h. Considered catalogs are not enough to consider larger scales but there was found no evidence of uniformity up to 100 Mpc/h.

References

1. Sylos Labini F.; Tekhanovich D.I.; Baryshev Yu. V. // JCAP vol. 7, p. 35 (2014).
2. Gabrielli A., Sylos Labini F., Joyce M., Pietronero L. Statistical Physics for Cosmic Structures – Springer, 2005 p. 91.

Estimation of Lamé parameters for the two-dimensional elasticity equations

Valitov Aleksandr
alexan.valit@yandex.ru

Scientific supervisor: Dr. Kashtan B.M., Department of Earth's Physics, Faculty of Physics, Saint-Petersburg State University

The solving of inverse problems is one of the main goals of modern science and especially in geophysics. The aim of the present work is realization of the inverse problem solving by the adjoint-state method (ASM) [1] for computing the gradient of an error functional. Estimating the model parameters from measured data generally consists of minimizing an error functional. Lamé parameters and density were chosen as the model parameters in this case. The goal of this work is to study and implement ASM in case of two-dimensional elasticity equations. Our virtual experiment shows on principle opportunity of using it in real experiment.

References

1. Plessix R.-E. // Geophys. J. Int. 2006. V. 167. P. 495-503.

C. Mathematics and Mechanics

Local bifurcation for discrete-time non-autonomous systems connected with a heart model

Abdalova Iuliia
yuliannia@gmail.com

Scientific supervisor: Prof. Dr. Reitmann V., Chair of Applied Cybernetics, Faculty of Mathematics and Mechanics, Saint-Petersburg State University

Results in bifurcation theory for autonomous differential and difference equations are well-known. For the investigation of such equations one typically applies a theorem of Shoshitaishvili using the Jacobi matrix of the system. But in the non-autonomous case, this theorem is not applicable. For non-autonomous differential equations first bifurcation results are proved in [1-3].

In the present work we introduce a modified principle of reduction for systems depending on a parameter. Using this principle we consider three basic types of bifurcations in discrete-time non-autonomous systems: the saddle-node, pitchfork and period-doubling bifurcations. Stability properties of the solutions of these systems are shown and analogies with autonomous discrete-time systems under certain conditions on the coefficients are demonstrated.

As an example we consider a two-dimensional non-autonomous discrete-time system which is used as a conduction model of the heart. Under certain typical assumptions for this system, we consider the equation expressing the dependence of the current conduction time and from a previous recovery time in a simplified form. We observe the behavior of this equation in the case of a constant control parameter which leads to so-called alternation which is connected with asphyxia, a heart diseases, described in [4].

References

1. Kloeden P.E., Siegmund S. // International Journal of Bifurcation and Chaos, v. 15, № 3, pp. 743-762 (2005).
2. Nguyen V. M. // Proceeding of the Royal Society of Edinburg, v. 123A, pp. 621-632 (1993).
3. Langa J., Robinson J.C. and Suarez A. // Nonlinearity, v. 15, pp. 1-17 (2002).
4. Sun J., Amellal F., Glass L. and Billette J. // J. Theor. Biol., v. 173, pp. 79-91 (1995).

Topology preserving algorithm for cartographic generalization

Alexeev Vladislav, V. Bogaevskaya, A. Gorokhov, V. Knyazev,
M. Preobrazhenskaia, A. Ukhalov, H. Edelsbrunner, O. Yakimova
thekinnbeetle@gmail.com

*Scientific supervisor: Dr. Yakimova O.P., Faculty of Mathematics,
Yaroslavl State University*

The object of this work is the problem of generalization of cartographic objects [1]. The source data for algorithm is a set of graphs embedded in the plane, each referred to as a layer. Each layer represents a particular cartographic object such as a country borders, rivers, roads etc. The aim is to simplify the data by decreasing the number of nodes of the graphs while preserving the global topology of the picture, which includes the relative position of objects to each other. The result of such a simplification can be used for representing the original map to given scale. The fundamental operation for simplifying the map is the edge *contraction* of an edge to a point. The position on the new vertex is chosen accordingly to the method described in [2]. The contraction of an edge can change the topology of the map, in which case we prevent the contraction. General conditions that recognize topology preserving edge contractions are given in [3].

Superimposing. We superimpose all the layers into one data structure. This allows us to simplify all layers simultaneously, thus preserving its global topology and not just the topology of each individual layer. We remember for each edge the original layer it belongs to.

Sorting. For each edge, we calculate the *cost* as the geometric error that results from contracting the edge [2]. Edges are stored in a priority queue ordered by cost so that edges can be contracted in the order of increasing cost.

Simplifying. We simplify the structure by contracting edge in the order of increasing cost. We stop when the number of vertices drops below a specified percentage of original number of vertices.

Smoothing. We finally smooth the resulting polylines with B-splines for improved appearance.

Decomposing. The simplified structure can now be decomposed into the individual layers, each a simplified version of the corresponding original layer.

The work was supported by the project No. 477 of P.G. Demidov Yaroslavl State University within State Assignment for Research.

References

1. A.M. Berlyant, O.R. Musin, and T.V. Sobchuk. Cartographic generalization and fractal theory. Moscow, 1998.
2. M. Garland and P.S. Heckbert. Surface simplification using quadric error metrics. SIGGRAPH '97, Proc. 24th Ann Conf. Comput. Graphics, 209 – 216.
3. T.K. Dey, H. Edelsbrunner, S. Guha and D.V. Nekhayev. Topology preserving edge contraction. Publ. Inst. Math. (Belgrad) (N.S.) 66 (1999), 23 – 45.

Controlling the controller: hysteresis-delay differential equations

Eyal Ron
eyalron33@gmail.com

***Scientific supervisor: Dr. Gurevich P., Faculty of Mathematics,
Freie University of Berlin***

Our talk revolves around differential equations with hysteresis and delay terms. We focus on the problem of stability analysis of periodic solutions. This problem is infinite-dimensional due to the delay and discontinuous due to the hysteresis. We reduce it, in certain cases, to an equivalent finite-dimensional problem. Our main application is a thermal control model. E.g, control precisely the temperature of a chemical reactor. It consists of a parabolic equation with hysteresis (controller) on the boundary. Gurevich and Tikhomirov recently showed the existence of both stable and unstable periodic solutions for such a model. Their result naturally raises the question of whether it is possible to change the stability properties of such solutions.

We use the well-known Pyragas control to change the stability of periodic solutions of the thermal control model. Using this method, one adds an additional delay term to the boundary without destroying the known periodic solution. This results in a parabolic equation with both hysteresis and delay terms on the boundary.

Using Fourier decomposition, this equation is reduced to a system of ODEs. Then we can apply our finite dimensional reduction technique and show that Pyragas control can change stability of periodic solutions.

Andronov–Hopf bifurcation in equation with inconstant delay

Golubenets Vyacheslav
golubenets2010@yandex.ru

*Scientific supervisor: Dr. Kashchenko I.S., Faculty of Mathematics,
Yaroslavl State University*

In this work we consider the equation

$$\dot{u} + u = bu(t - T(u)), \quad (1)$$

where b is a parameter, $T(u)$ is certain everywhere positive and bounded function. We use the $u = \psi(t)$ as initial condition for equation (1), where $\psi(t)$ is continuous function defined on the interval $[-T_1, 0]$. T_1 is the maximum value of $T(u)$.

The problem is to investigate the behavior of solutions of the equation (1) in a small neighbourhood of its zero equilibrium state. It's known there is $b=b_0$ such that if $b \in (b_0, 1)$ then zero solution of equation (1) is stable; if $b < b_0$ or $b > 1$ then it is unstable; values $b = b_0$ and $b = 1$ are bifurcation's values.

Consider $b = b_0 + \varepsilon$, where ε is sufficiently small. So we study the case that is close to critical.

The method we use for solving the problem is the method of normal forms. Its main idea is to obtain a new equation by using the special change of variables in equation (1). This new equation is the simplest form of equation (1) and called the normal form of (1). The normal form is easier to research and the dynamics of its solutions is coincides with the dynamics of solutions of equation (1) in a small neighbourhood of an equilibrium state.

After using this method we obtain a sufficient condition for the function $T(u)$ under which the supercritical Andronov–Hopf bifurcation takes place in initial equation.

Andronov-Hopf bifurcation of one or more cycles in the Mackey-Glass type delay differential equation

Ignatenko Vera
veraignatenko93@gmail.com

Scientific supervisor: Prof. Dr. Reitmann V., Department of Applied Cybernetics, Faculty of Mathematics and Mechanics, Saint-Petersburg State University

We consider the parameter-dependent model of Mackey-Glass with time-delay nonlinearity [1]. Such model describes the regulation of hematopoiesis (a process of blood cell production).

Using the finite-dimensional version of the Andronov-Hopf bifurcation theorem [2] we derive conditions for the parameters under which the creation of exactly one limit cycle is possible. In particular, we suppose here that the first Lyapunov value is different from zero.

Furthermore, we investigate the reduced bifurcation equation in the case when the first Lyapunov value is zero. This leads [3] to the possibility of the bifurcation of two cycles in the system.

References

1. M.C. Mackey, L. Glass // Oscillations and Chaos in Physiological Control Systems. Science, New Series, v. 197, № 4300, p. 287-289 (1977).
2. B.D. Hassard, N.D. Kazarinoff, Y.-H. Wan // Theory and Applications of Hopf Bifurcation. London Mathematical Society Lecture Note Series 41, Cambridge University Press (1981).
3. J.K. Hale // Behavior near constant solution of functional differential equations. Journal of Differential Equations, v. 15, p. 278-294 (1974).

Homogenization of the first initial-boundary value problem for parabolic systems: L_2 -operator error estimates

Meshkova Yulia
juliavmeshke@yandex.ru

Scientific supervisor: Prof. Dr. Suslina T.A., Department of Higher Mathematics and Mathematical Physics, Faculty of Physics, Saint-Petersburg State University

The talk is devoted to homogenization of periodic differential operators. We study the behavior of the solutions of the first initial-boundary value problem in a bounded domain Ω . In operator terms, we deal with the exponential $\exp(-A_\varepsilon t)$, $0 < \varepsilon \leq 1$, $t > 0$. Here A_ε is the self-adjoint second order differential operator acting in $L_2(\Omega)$. The coefficients of A_ε are periodic with respect to some lattice and depend on x/ε . So, the coefficients oscillate rapidly for small ε .

To describe the behavior of $\exp(-A_\varepsilon t)$, we introduce the effective operator A^0 . It is an operator with constant coefficients. Definition of the effective operator is well-known in homogenization theory.

Our main result is as follows. For a fixed time $t > 0$, the operator $\exp(-A_\varepsilon t)$ converges to $\exp(-A^0 t)$ in the L_2 -operator norm. For the difference of the exponentials we have obtained an estimate of the precise order ε . The constants in this estimate are controlled explicitly in terms of the problem data. Results of this type are called operator error estimates in homogenization theory. Results about the operator exponential are applied to homogenization of the first initial-boundary value problem.

The method of investigation is based on the representation for the exponential $\exp(-A_\varepsilon t) = -(2\pi i)^{-1} \int_\gamma \exp(-\zeta t) (A_\varepsilon - \zeta)^{-1} d\zeta$. Here γ is a suitable contour in the complex plane. For $\exp(-A^0 t)$ we have a similar identity. Thus, the problem reduces to approximation of the resolvent $(A_\varepsilon - \zeta)^{-1}$ obtained by Suslina T.A. [1].

The talk is based on a joint work with Suslina T.A. [2].

This research is supported by the Chebyshev Laboratory (Department of Mathematics and Mechanics, St. Petersburg State University) under RF Government grant 11.G34.31.0026 and JSC "Gazprom Neft".

References

1. Suslina T.A. Homogenization for the elliptic problems in dependence of the spectral parameter // *Funct. Anal. Appl.*, to appear.
2. Meshkova Yu.M., Suslina T.A. Homogenization for the solutions of initial-boundary value problems for parabolic systems // *Funct. Anal. Appl.*, to be published.

Numerical probabilistic approach to solution of the Cauchy problem for quasilinear parabolic equations

Nemchenko Ekaterina
nemchenko_ekaterina@mail.ru

Scientific supervisor: Prof. Dr. Belopolskaya Y.I., Department of Mathematics, Civil Engineering Faculty, Saint-Petersburg State University of Architecture and Civil Engineering

Quasilinear parabolic equations of the form

$$\frac{\partial u}{\partial t} + \frac{1}{2} \text{Tr}[A^*(x, u, \nabla u) \nabla^2 u A(x, u, \nabla u)] + a(x, u, \nabla u) \cdot \nabla u + g(x, u, \nabla u) = 0, \quad (1)$$

arise as mathematical models of various phenomena in physics, biology, financial mathematics and other fields. Probabilistic approaches to solution of such problems are well developed [1, 2].

The aim of this work is to construct and implement a numerical algorithm for solving equations of the form (1) with the Cauchy data

$$u(T, x) = u_0(x), \quad x \in R^d, t \in [0, T], \quad (2)$$

based on a probabilistic representation of the solution of the problem (1), (2).

We assume that $u_0(x)$ is a bounded function, coefficients a, A and g are sublinear and satisfy the Lipschitz condition in all arguments.

Let $w(s) \in R^d$ be a standard Wiener process defined on a probability space

$$(\Omega, F, P) \text{ and } z \cdot w = \sum_{k=1}^d z_k w_k.$$

Consider a system of stochastic equations, consisting of a forward SDE

$$d\xi(s) = a(\xi(s), y(s), z(s))ds + A(\xi(s), y(s), z(s))dw(s), \quad \xi(t) = x \quad (3)$$

where $0 \leq t \leq s \leq T$, and a backward SDE (BSDE)

$$dy(s) = g(\xi(s), y(s), z(s))ds + z(s) \cdot dw(\theta), \quad y(T) = u_0(\xi(T)). \quad (4)$$

A solution $y(s) = u(s, \xi(s)), z(s) = A^*(\xi(s), y(s), z(s)) \nabla u(s, \xi(s))$ of (4) with $\xi(s)$ satisfying (3) via relation $y(t) = u(t, x)$ gives rise to a continuous viscosity solution of the Cauchy problem (1), (2). Thus, solving numerically system (3), (4), we construct a numerical solution of the problem (1), (2).

References

1. Ya. Belopolskaya // Global and Stochastic Analysis, v. 1, № 1, p. 3-402, (2011).
2. S. Peng, M. Xu // ESAIM: Mathematical Modelling and Numerical Analysis, v. 45, Issue: 2, pp. 335 – 360, (2011).

Shadowing for systems without transversality

Petrov Aleksey
al.petrov239@gmail.com

Scientific supervisor: Prof. Dr. Pilyugin S.Yu., Department of Higher Geometry, Faculty of Mathematics and Mechanics, Saint-Petersburg State University

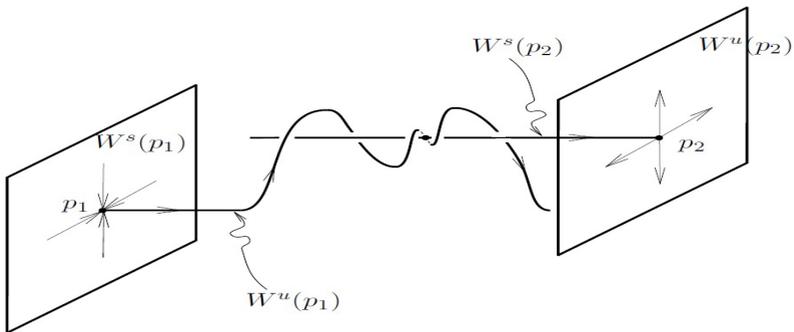
The notions of a pseudotrajectory and shadowing property of a homeomorphism play an important role in the general qualitative theory of dynamical systems.

From the numerical point of view, if a homeomorphism has the shadowing property, then the behavior of all numerically obtained trajectories coincides with the behavior of real trajectories.

It is well known that for a diffeomorphism f of a closed manifold M , the following three conditions are equivalent: (1) f has the shadowing property (and this property is Lipschitz); (2) f satisfies Axiom A and the strong transversality condition; (3) f is structurally stable.

In [1], Sakai proved that a two-dimensional system with Axiom A has the shadowing property if and only if it satisfies the so-called C_0 -transversality condition. So it seems very natural to study systems with Axiom A and to try to formulate for such systems necessary and sufficient conditions of shadowing in terms of some transversality condition.

However, in our talk we will discuss an example of a system with Axiom A that has the shadowing property but fails to satisfy any transversality condition.



References

1. K. Sakai, Shadowing property and transversality condition, *Dynamical Systems and Chaos* (World Sci., Singapore, 1995), Vol. 1, pp. 233-238.

Control of synchronization in neural delay-coupled networks with heterogeneous threshold parameters

Plotnikov Sergei
waterwalf@gmail.com

Scientific supervisor: Prof. Dr. Fradkov A.L., Department of Theoretical Cybernetics, Faculty of Mathematics and Mechanics, Saint-Petersburg State University

. The ability to control nonlinear dynamical systems has brought up a wide interdisciplinary area of research that has evolved rapidly in the past decades. On the other hand, the study of networks has gained increasing importance due to its widespread applicability in such areas as social sciences, computer science, economics, biology, physiology, and ecology. In the analysis of network dynamics, synchronization is a field of high interest. An efficient way to synchronize the system is the use of adaptive control.

In this work the network of FitzHugh-Nagumo systems with heterogeneous threshold parameters is considered. It is a more common case of such system. The FitzHugh-Nagumo model is paradigmatic for excitable dynamics close to a Hopf bifurcation. The bifurcation analysis is made, and conditions for bifurcation occurrence are given. For synchronization achievement the speed-gradient algorithm is applied, which was used previously in various nonlinear control problems, even for the control of dynamics in delayed-coupled networks.

Monte Carlo Simulation for Stochastic Differential Equations

Pogosian Anna
anna.a.pogosian@gmail.com

Scientific supervisor: Prof. Dr. Ermakov S.M., Department of Statistical Modelling, Faculty of Mathematics and Mechanics, Saint-Petersburg State University

Monte Carlo Method is often used as a powerful and efficient tool for solving integral equations of the second kind [1].

A differential equation, including nonlinear case and system of equations, can be easily converted into an integral equation of the second kind.

A numerical estimate for the solution of the converted equation can be obtained from a number of Monte Carlo simulations based on a model of a branching process.

Said technique can be applied to stochastic differential equations.

A number of estimates for solutions and numerical examples in accordance with the aforementioned technique are provided in the report.

References

1. Ермаков С.М. Метод Монте-Карло в вычислительной математике. Вводный курс. СПб: «Невский диалект»; Москва: «Бином», 2009. 94 с.

Application of the Method of Quasi-Normal Forms to the Mathematical Model of a Single Neuron

Preobrazhenskaia Margarita
rita-uvarova@yandex.ru

Scientific supervisor: Dr. Kolesov A.Y., Department of Differential Equation, Faculty of Mathematic, Yaroslavl State University

The object of investigation of this work is a scalar nonlinear differential-difference equation with two delays

$$\dot{u} = \lambda \left((a + 1)f(u(t - h_1)) - a - bg(u(t - h_2)) \right) u. \quad (1)$$

It models the behavior of a single neuron. Here $u(t) > 0$ is the neuron's membrane potential, the parameter λ describes the rate of electrical processes in the system and assumed to be large, h_1, h_2, a, b are the positive parameters. The functions $f(u), g(u)$ belong to class $C^\infty(\mathbb{R}_+)$, where $(\mathbb{R}_+) = \{u \in \mathbb{R} : u > 0\}$. This equation was first introduced in [1] based on the model of a single neuron, which is described in [2]. Later it was considered in the number of papers, for example in [3, 4].

Under certain additional conditions on the functions $f(u)$ and $g(u)$, the equation (1) has the unique equilibrium state $u = u_0(a, b)$. We pose the question of its stability by changing parameters b, h_1, h_2 . More precisely, as in [3] we are interested in singularly perturbed case, when

$$\frac{h_1}{h_2} = \varepsilon h, \quad h = \text{const} > 0, \quad \varepsilon = \frac{1}{\lambda}, \quad 0 < \varepsilon \ll 1.$$

Under a suitable choice of parameters b and h the well-known method of quasi-normal forms is applied to this equation. The result of its application is the boundary value problem type Korteweg - de Vries equation. The investigation of this boundary value problem allows us to conclude about the behavior of the original equation. Namely, for a suitable choice of parameters the buffer phenomenon is realized in the equation (1). It means that the equation has arbitrarily large number of stable cycles.

References

1. S.D. Glyzin, A.Yu. Kolesov, N.Kh. Rozov // Mathematical Notes, 2013, 93:5, 676-690.
2. S.A. Kashchenko, V.V. Maiorov. Modeli volnovoy pamyati. -M.: Knizhnyy dom LIBROKOM, 2009. [in Russian].
3. S.D. Glyzin, A.Yu. Kolesov, N.Kh. Rozov // Buffer phenomenon in neurodynamics, Doklady Mathematics. 2012. V.85. No. 2. P. 297-300.
4. S.D. Glyzin, A.Yu. Kolesov, N.Kh. Rozov // Computational Mathematics and Mathematical Physics, 2012, 52:5, 702-719.

Simulations of high-velocity star motions in the Galactic gravitational field

Shirokova Kseniia
xebusk@mail.ru

Scientific supervisor: Prof. Dr. Orlov V.V., Department of Celestial Mechanics, Faculty of Mathematics & Mechanics, Saint-Petersburg State University

Discovered not so long ago hypervelocity stars are new, the fastest class of high-velocity objects in the Galaxy. However, their origin remains unclear.

The first proposed by Hills [1] mechanism of interaction between a close binary system [2] and a supermassive black hole has been modeled using a model potential of the Galaxy [3]. 1000 variants of the initial velocities were considered for three different variants of the initial closeness of encounter of a binary system with a black hole.

Obtained by modeling the data qualitatively agree with the observations, but available observational data are insufficient for an unambiguous confirmation of this hypervelocity stars formation method.

References

1. J.G. Hills // Nature 331, 687 (1988).
2. G.N. Dremova, V.V. Dremov, A.V. Tutukov // Astronomy Reports 58, 291 (2014).
3. M. Fellhauer, V. Belokurov, N.W. Evans, M.I. Wilkinson, D.B. Zucker, G. Gilmore, M.J. Irwin, D.M. Bramich, S. Vidrih, R.F.G. Wyse, T.C. Beers, J. Brinkmann // Astrophys. J. 651, 167 (2006).

Preprocessing of endoscopy images

Symanovich Maksim
MAXbrainRUS@gmail.com

Scientific supervisor: Dr. Dunaeva O.A., Department of Computing and Programming Systems, Faculty of Information and Computer Science, Yaroslavl State University

High-magnification endoscopy with narrow-band imaging (HME-NBI) has been used for diagnosis of gastric pathology. We developed the computer-aided system for classifying endoscopic images and improving the accuracy of medical diagnosis. Endoscopic images have a few features that should be taken into account in processing: the poor resolution, patient information displayed on some part of image, the lighting is not uniform, and the image has reflections. This article is about methods of preprocessing endoscopic image such as a selection of informative area, specular reflections detection, and the brightness image equalization.

Selection of informative area. On the endoscopic image we have a octagonal area with gastric mucosa, the size and position of this region depend on endoscopic equipment. Note that we have significant changes of brightness on the boundary of this area. We detect boundary points using the threshold binarization of image gradient. After that, we apply the optimization methods for selecting parameters of the octagon model.

Specular reflection detection. We convert source image from RGB to the HSB (hue, saturation, brightness) color model. We can recognize specular reflections by checking whether $s < s_0$ and $b > b_0$, for suitable constants s_0 and b_0 ; see [1]. We use $s_0 = 0.2$ and $b_0 = 0.9$ in this paper.

Brightness equalization. We have different illumination for different areas of image. We calculate the average value of brightness of the point as median value of brightness of points inside a square window with a center at this point. To suppress the effect of uneven illumination of the image, we change the value of each point of the image by subtracting the average brightness of this point.

Subsequent endoscopic image processing includes calculating the vector of descriptors which used for training of the classifier. The first and second stages of preprocessing allow to exclude uninformative areas from the future analysis. It's important because they worsen the quality of descriptors. In some sense the brightness equalization normalize the value of calculated descriptors. In particular, the use of brightness equalization algorithm has greatly improved the results of the classifier constructed on topological features.

References

1. Stehle T., Auer R., Gross S., Behrens A., Wulf J., Aach T., Winograd R., Trautwein C., Tischendorf J. Classification of colon polyps in NBI endoscopy using vascularization features // Medical Imaging 2009: Computer-Aided Diagnosis, eds. N. Karssemeijer and M. L. Giger, SPIE, 7260, 2009.

Caratheodory dimension of invariant sets for dynamical systems with multiple time

Voynov Dmitriy
voynov@math.spbu.ru

Scientific supervisor: Prof. Dr. Reitmann V., Chair of Applied Cybernetics, Faculty of Mathematics and Mechanics, Saint Petersburg State University

A dynamical system with multiple time (DSMT) is a generalization of a standard dynamical system, i.e. system with one dimensional time. Such DSMT are generated by partial differential equations and Pfaffian systems. They have applications in differential geometry, mathematical physics and other fields [1].

For standard dynamical systems special outer Caratheodory measures are constructed in [2, 3]. These outer measures give the opportunity to estimate Hausdorff measures and Hausdorff dimension of attractors for standard dynamical systems.

We use analogous methods for the construction of Caratheodory structure in a form of so called containers for dynamical systems with multiple time [4].

References

1. Gaishun I.V. // Completely Integrable Multidimensional Differential Equations. (In Russian). -Moscow: Nauka i tekhnika, 1983, -258 pp.
2. Boichenko V.A., Leonov G.A., Reitmann V. // Dimension Theory for Ordinary Differential Equations. -Wiesbaden: Teubner, 2005, -405 pp.
3. Leonov G.A. // Vestnik of Saint Petersburg State University, v.1, №.4, pp. 24-31 (1995).
4. Voynov D.A. // Caratheodory dimension structure for general dynamical systems. (In Russian). Year project, Saint Petersburg State University, pp. 1-10. (2014).

E. Applied Physics

Gas-separating membranes based on polyimides of variable structure

Antipov Mikhail
posich@mail.ru

Scientific supervisor: Dr. Yevlampieva N.P., Polymer Physics Department, Faculty of Physics, Saint-Petersburg State University

Membrane forming polymers are widely used now in the industry. For instance, as the selective filters for cleaning and division of preparations in medicine, pharmacology and biotechnologies, as the barrier-materials in production of power supplies, accumulators and batteries for electronic devices, as gas-selective membranes in recycling chemical processes, etc. [1]. One of the modern trends in the field of polymeric membranes is a searching of novel highly selective membrane polymers for separation of hydrogen from hydrogen-containing gas mixtures. As it was shown not far ago [2], polyimides are one of the most suitable class of polymers that may be utilized for the manufacture of gas-permeable membranes. They exhibit a high chemical and thermal stability and good mechanical and film-forming properties.

A present work is devoted to study of heat-resistant membranes for a preliminary cleaning and division of synthesis-gas used in hydrogen energetic. Gas-permeability and gas-separation characteristics of membranes on the basis of polyimides of different chemical structure were investigated and compared to composite polyimides. The polymeric films of 15-45 microns thickness was used to receive a reliable data on definition of fundamental gas transmission characteristics at temperature interval 20-150 °C and at pressure range 0-8 atm. Our study had shown that a composite membrane material based on polyimide possess a significantly higher rate permeation/selection in comparison with the initial polymer.

References

1. Richard W. Baker. Membrane technology and applications. – Wiley.: London–2000. p.588.
2. Alentiev A. Y., Loza K. A., Yampolskii Y. P. // J. Membr. Sci. – 2000. – V. 167. – № 1. – P. 91-106.

Effect of the solution parameters on the characteristics of the Ag nanoparticles obtained by method of direct laser synthesis

Leonova Iuliia
yulchik-leon@yandex.ru

Scientific supervisor: Dr. Manshina A.A., Department of General Physics-1, Faculty of Physics, Saint-Petersburg State University

Noble metal nanoparticles acquire a great interest because of the plasmon resonance phenomenon, which is used in various fields of science and technology. The silver nanoparticles also have other important properties so that they could be used, for example, as antibacterial agents or as a part of fluorescent markers for cancer diagnosis. Due to the development of new methods of synthesis of the particles a simple and effective method of direct laser synthesis of silver nanoparticles has been recently proposed. It is that under the action of laser radiation focused in the solution, the chemical reaction proceeds and produces nanoparticles [1]. The scope of the reaction is limited by the focus area of the laser beam, whereas the time is limited by the pulse duration. It determines the conditions for the formation of nanoscale Ag particles.

In this study we tried to evaluate the influence of the parameters of the used solution on the characteristics of the obtained silver nanoparticles. The three solution formulas were used: ammonia-alcohol solution AgNO_3 , aqueous solution CH_3COOAg , AgNO_3 solution in an aqueous solution of urea, and 4 concentrations of each composition in a ratio of 1:2:3:4. It has been found that obtaining of nanoparticles is possible in case of using ammonia-alcoholic solution of AgNO_3 , and their size and optical properties depend on the concentration of the used solution (Fig. 1). It has been also found that in each case there is a narrow particle size distribution, especially in the case of the lowest concentration 0,1 mole / liter - 23 to 29 nm.

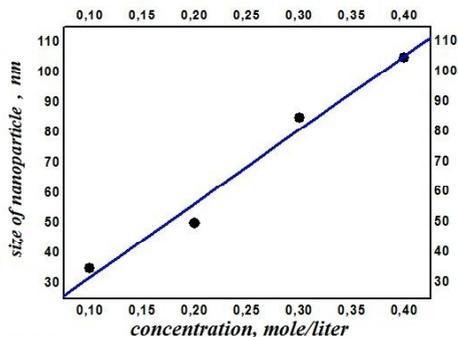


Fig.1. Dependence of the size of the resulting Ag nanoparticles on the concentration used ammonia-alcohol solution

References

1. T. Nakamura, H. Magara, Y. Herbani, and S. Sato. Fabrication of silver nanoparticles by high-intensity of laser irradiation of aqueous solution / ALC'09, 10P10, Maui – Hawaii, pp. 507–510, 2009.

Light control over plasmon properties of gold nanoparticles

Lysyakova Liudmila
lysyakov@uni-potsdam.de

*Scientific supervisor: Prof. Dr. Santer S., Experimental Physics,
Institute of Physics and Astronomy, University of Potsdam*

Photosensitive azonbenzene containing surfactants have attracted considerable interest due to their versatile applications in the field of light controlled shape and functionality of soft nano-objects [1, 2]. Photosensitive surfactant consist of charged head group and hydrophobic chain with integrated azobenzene group. Azobenzene unit is known to undergo trans-cis isomerization under irradiation with light, serving therefore a photo-trigger for the hydrophobicity of the surfactant. The complex formation between laser ablated gold nano-particles (10 nm average diameter) and photosensitive azobenzene containing cationic surfactant was studied by UV-Vis absorption spectroscopy, dynamic light scattering and electron microscopy.

The interaction with the surfactants strongly alters plasmon properties of the gold nano-particles. The position of gold plasmon peak shifts from 523 nm for bare gold nano-particles to 527 nm for nano-particles decorated with surfactant molecules. Depending on gold-surfactant molar ratios three different constitutions of the nano-particle/surfactant complexes were identified. In the region I and III, at low and high surfactant-to-gold molar ratios, respectively, the nano-particles are represented by single specimens either negatively (region I) or positively (region III) charged. In the intermittent region II the nano-particles being turned hydrophobic by attached surfactant molecules form conjugates of around 100 nm in diameter. In this region, the second absorption peak at $\lambda > 650$ nm appears, what is visually detectable by change in the solution color from red to blue. We have shown that using UV light it is possible to induce transition of the gold-surfactant complex configuration from the region III of single nano-particles to the region II of gold nano-clusters without altering absolute value of the surfactant concentration.

References

1. Zakrevskyy, Y.; Kopyshv, A.; Lomadze, N.; Morozova, E.; Lysyakova, L.; Kasyanenko, N.; Santer, S. // *Phys. Rev. E*, 84, 021909 (2011).
2. Zakrevskyy, Y.; Roxlau, J.; Brezesinski, G.; Lomadze, N.; Santer, S. // *Chem. Phys.*, 140, 044906 (2014).

Research of consequences of the accidents at nuclear power plants and impact on the environment of Leningrad region

Merzlaya Anastasia
stummeworte@mail.ru

Scientific supervisor: Dr. Torilov S.Yu., Department of Nuclear-Physics Research Methods, Faculty of Physics, Saint-Petersburg State University

The most adverse consequences of nuclear power engineering are catastrophes happened at nuclear power plants and the distribution of released radionuclides and environmental pollution. As a result of these accidents released radionuclides from discarded nuclear reactor materials spread around the world. For example, after the accidents occurred in the Chernobyl and the Fukushima released more than 10 thousand PBq.

In the work the experimental data of research of background soil samples taken from the Eastern part of the Leningrad region were produced. Investigation was carry out using semiconductor HPGe gamma-detector, that was surrounded by a lead shield, with the relative efficiency 20% and energy resolution 1.8 KeV at the peak of ^{60}Co 1333 KeV. Measurement of the background in the Old Peterhof (Leningrad region) showed that in the spectrum except for the lines of primordial single radionuclides and radioactive series observed peak of artificial radionuclide ^{137}Cs , which was identified as having the Chernobyl origin according its half-decay period; the peak of ^{134}Cs , which can identify the Fukushima trace, doesn't exceed 0.01 Bq.

For a more detailed study of the pollution of the environment topsoil samples from the Eastern part of the Leningrad region were measured. The results showed occurrence of ^{137}Cs over the background practically in all samples. Moreover, a significant expansion of the border of radioactive zones, determined according earlier investigation using scintillation spectrometer [1], was noticed. So the activity of ^{137}Cs of the samples from the contaminated area according [1] is approximately $200 \text{ Bq}\cdot\text{kg}^{-1}$, but there are places outside the polluted zones with the activity of ^{137}Cs is more than $300 \text{ Bq}\cdot\text{kg}^{-1}$. The map [1] can be corrected using the obtained data in the study region.

References

1. Leningrad region. The map of the radioactive contamination of the area (by ^{137}Cs). SPb, "TECHCO", 1992.

Manipulation azobenzene containing surfactant via far – and nearfield

Johann Nuck,¹ Burhard Stiller,¹ Yuri Petrov², Vladimir Mikhailovskii², Oleg Vyvenko,² Svetlana Santer¹
jnuck@uni-potsdam.de

Scientific supervisor: Prof. Santer S., Institute of Physics and Astronomy, University of Potsdam, Germany

¹ *Institute of Physics and Astronomy, University of Potsdam, Germany,*

² *Interdisciplinary Resource Center for Nanotechnology, Saint Petersburg State University, Russia*

Controlled adsorption and structuring of molecularly thin polymer films or ensembles of nanoparticles on solid substrates is still a major challenge in nanotechnology. With our study, we aim at developing a novel approach of how charged species such as polyelectrolytic polymers and colloids can conveniently and quickly be spatially organized according to an externally imposed light density distribution provided e.g. by a suitably interference pattern. For this purpose we prepare a self assembled monolayer (SAM) of azobenzene containing molecules covalently bonded to a gold and a silver surface. Azobenzene unit undergoes photoisomerisation reaction under UV irradiation resulting in a change in the dipole moment of the molecule. Our approach allows for fabrication of stimuli responsive surfaces with locally varying surface properties such as surface energy or/and surface chemistry. The change in surface properties is induced and triggered by light as external stimuli.

We studied three types of the molecules differing in the nature of the end group to be CF_3 , CH_3 or SO_2 . The photoisomeriation was induced using both far field interference pattern and surface plasmons near field pattern. In order to generate far field interference pattern, 2-beam interference lithography with a laser of 442 nm wavelength was used. The surface plasmons (SP) were excited within a nano-structured metallic mask milled by focused ion beam. The generated SP can propagate and interfere resulting in standing waves bound to a surface. Using a Kelvin probe we have observed that photoisomerisation can be induced by both far field and SP near fields. Also local structuring of the SAM was produced after irradiation with 442 nm. The stripes of different surface energy were generated within the SAM, while the topographical changes were not detected.

Study of the characteristics of neutron scintillators

Safiulina Irina
ira93@inbox.ru

Scientific supervisor: Dr. Ilyin D.S., Petersburg Nuclear Physics Institute

Detectors for neutron registration, which are most widely used at present, can be classified in two basic classes: the gas-filled detectors and scintillation detectors.

Recently scintillation detectors have attracted a lot of attention. This is due both to the specific unique characteristics of scintillation detectors and deficient isotope of helium (^3He), which is the most common converter for neutrons in the gas-filled detectors, accounting for the major share the gas mixture [1].

In the experiment were studied 4 scintillators: 2 lithium glasses with different contents trivalent cerium, borate glass and scintillation screen ZnS/LiF. For each of them was obtained the emission spectrum and the absorption spectrum in order to identify the most effective scintillator, which will have the greatest light output.

In the experiment it was found that the scintillation screen ZnS/LiF has the highest light output (Fig. 1). Then the sample has been studied in the reactor. It was that the feature of scintillation screen ZnS/LiF is different time of emission of gamma and neutron impulses. Using the method of separation of these pulses, in the future we can estimate the neutron registration efficiency detector.

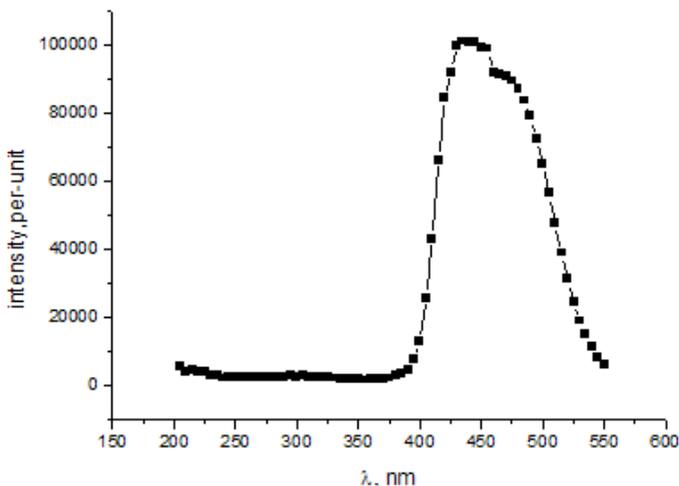


Fig. 1. Light output of scintillation screen ZnS/LiF.

References

1. Thomas K. McKnight // Master's thesis (2005).

Manufacturing and testing an electrochemical cell for the anodic oxidation of titanium

Starodubtseva Lyudmila
lyudmilastar@list.ru

*Scientific supervisors: Prof. Dr. Emelin A.V., Murash-kina A.A.,
Faculty of Physic, Saint-Petersburg State Uni-versity*

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. Last process plays a key role in exploration of the mechanisms of photoinduced surface reactions [1].

Today, it is shown that almost any organic compound can be oxidized to CO_2 and H_2O on the TiO_2 surface. If the composition includes compounds of nitrogen or halogen atoms X, then HNO_3 and HX will be observed in the reaction products. The only known example of a compound that does not undergo oxidation on the surface of TiO_2 , is carbon tetrachloride [2]. However, the production of nanotube arrays by electrochemical anodization of the parent metal provides excellent control over nanotube growth [3].

In the present work we created electrochemical cell (Fig. 1):

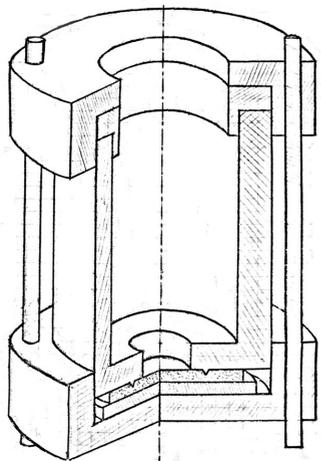


Fig. 1. Scheme of the working cell.

References

1. Tetsuya Kisumi, Akira Tsujiko, Kei Murakoshi, Yoshihiro Nakato, //Journal of Electroanalytical Chemistry 545 2003.
2. Булдаков Д.А. Плёнки анодного оксида титана как прототип мембран для фотокаталитической очистки воды. - Москва, 2009 год.
3. Sanju Rani, Somnath C.Roy, Maggie Paulose, Oomman K. Varghese, Gopal K. Mor, Sanghoon Kim, Sorachon Yoriya, Thomas J. LaTempa and C.A. Grimes // Physical chemistry chemical physics, 2010.

Velocity spread in quantum hydrodynamics

Zippa Andrey
andreyzippa@yandex.ru

Scientific supervisor: Prof. Dr. Ivlev L.S., Department of Atmosphere Physics, Faculty of Physics, Saint-Petersburg State University

Quantum hydrodynamics as a convenient method for solving the Schrödinger equation has been developed David Bohm and others [1]. Main feature of this method is definition of velocity $\vec{v} = \nabla S / m$ via phase of wave function. In case of a potential field, 3rd order linear equation for a wave length $\lambda = 2\pi\hbar / mv$ of a particle can be derived [2]. In homogeneous bounded electric field the “quantum velocity” vs. distance x is expressed via the Airy functions:

$$V_{quant}(x) = \frac{const}{Ai^2 \left[-\left(\frac{2meE}{\hbar^2}\right)^{1/3} \cdot x - \left(\frac{2meE}{\hbar^2}\right)^{-2/3} \cdot \frac{m^2 v_0^2}{\hbar^2} \right] + Bi^2 \left[-\left(\frac{2meE}{\hbar^2}\right)^{1/3} \cdot x - \left(\frac{2meE}{\hbar^2}\right)^{-2/3} \cdot \frac{m^2 v_0^2}{\hbar^2} \right]}$$

Using quantum hydrodynamics and classical mechanics, calculations were made (Fig. 1) for protons (mass m , charge e) with initial velocity $v_0 = 450$ km/s (mean one of the solar wind) passing through homogeneous electric field of strength $|E|=130$ V/m, like the natural electric field of the Earth. The velocity spread is the difference of the quantum and classical velocities

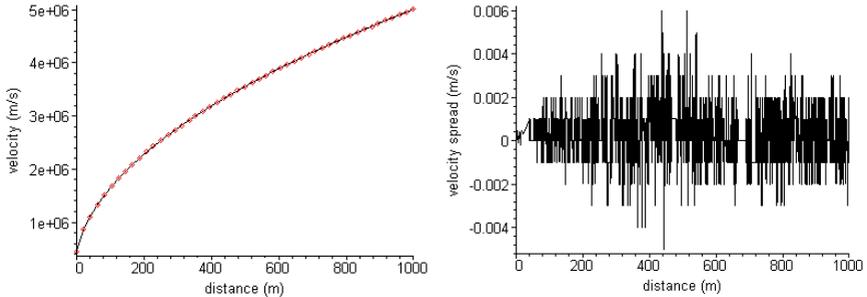


Fig. 1. Movement of the protons in the homogeneous electric field. Left: velocity of protons in quantum hydrodynamics (points) and classical mechanics (line), Right: velocity spread in quantum hydrodynamics.

References

1. R. Wyatt. Quantum dynamics with trajectories: introduction to quantum hydrodynamics. Springer (2005).
2. A.I. Zippa // Vestnik SPbGU, ser. 4, № 3, p. 21-26 (2011). In Russian.

D. Solid State Physics

Nuclear spin relaxation in bulk and nanostructured sodium

Antonenko Anastasiia
nastyas555@mail.ru

Scientific supervisor: Prof. Dr. Charnaya E.V., Department of Solid State Physics, Faculty of Physics, Saint-Petersburg State University

NMR methods are successfully used to study the mobility in various liquids embedded into mesoporous matrices. However, despite numerous studies we don't have enough information about nuclear spin relaxation and dynamics in metallic melts under confinement. For example, measurements of the spin-lattice relaxation time for melted gallium and indium [1] embedded into the porous glass with pores of 8 nm and opals showed a remarkable increase in quadrupole relaxation due to slowing down the atomic mobility in confined geometry. Our aim is to study changes in the physical properties of metallic sodium embedded into a nanoporous matrix compared to the relevant bulk.

The measurements were run at room temperature. ^{23}Na relaxation for a sodium loaded porous glass with 3.5 nm pores was studied using two NMR spectrometers, Avance400 and Avance750, at different magnetic fields. Theoretical estimates show that the quadrupole contribution to spin relaxation is very small when one considers the bulk sodium and, therefore, relaxation is due to the magnetic coupling with conduction electrons. For confined sodium the quadrupole relaxation mechanism starts dominating. It was obtained that the value of the correlation time of atomic mobility at room temperature is $\tau_c = (8.6 \pm 0.7) \cdot 10^{-10}$ s which is much shorter than in bulk sodium. This result reveals a pronounced acceleration of self-diffusion in nanostructured solid sodium compared to bulk solid sodium. It should be emphasized that such studies are possible because of the cubic symmetry of crystalline sodium which prevents strong NMR line broadening caused by the anisotropy of the Knight shift in non-cubic metals.

References

1. E.V. Charnaya, C. Tien, M.K. Lee, Yu.A. Kumzerov Atomic mobility in nanostructured liquid Ga-In alloy // J. Phys.: Condens. Matter 22, 195108 (2010).

Simulation of quantum yields of heterogeneous processes

Bakiev Tair
tairbakiev@gmail.com

Scientific supervisor: Prof. Dr. Emelin A.V., Department of Photonics, Faculty of Physics, Saint-Petersburg State University

Photochemical reactions in heterogeneous systems are very important in applied physics. The most important parameter in the photochemical reaction is the quantum yield. Important is the study of the dependence of the quantum yield of the photochemical reaction of various system parameters and system configuration.

In this study, I propose a theoretical estimate of the quantum yield of the reaction using different models. Starting from the simple model with several plates, with a further complication, which takes into account the reflection and scattering of light from the surface, heterogeneity generation of charge carriers through the entire thickness of plates and their diffusion to the surface, using a solution of the continuity of equation.

On the basis of these models were formulas derived for estimating the quantum yield. According to the obtained formulas graphs of the spectral dependence of the quantum yield for some parameters of the system and depending on the quantum yield of the system parameters. The results obtained for these models were compared with experimental data.

Detailed formulas, graphs and calculations will be presented in the poster.

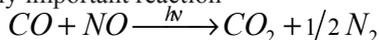
**"Self-sensitization" of Photocatalytic Activity of ZnO
into visible region for $CO + NO \xrightarrow{h\nu} CO_2 + 1/2 N_2$
reaction**

Blashkov Ilya
slipknoter90@rambler.ru

***Scientific supervisor: Prof. Dr. Lisachenko A.A., Department of
Photonics, Faculty of Physics, Saint-Petersburg State University***

TiO₂ and ZnO are the most widespread photoconverters of solar energy into chemical and electric one. However, these oxides exhibit their own absorption in UV wavelengths spectrum area, which amount less than 5% of sunlight radiation. For being used in visible area these oxides are sensibilized by different dyes, anions/cations of metals. Another way is to create oxides' composites with narrow zone semiconductors. In [1] the original self-sensitization method of the TiO₂ photocatalyst by own defects or creation of superficial 2D structures TiO₂/TiO_{2-x} is offered.

Research of possibility of "self-sensitization" of the ZnO photocatalyst on the example of ecologically important reaction



became the purpose of the study.

The spectral sensibility area of this photocatalytic reaction was significantly shifted from the UV edge (385 nm) of ZnO to the visible light area up to $\lambda > 570$ nm using intrinsic point defects of F-type. It is shown that kinetics details of photocatalytic reaction $NO + CO + h\nu \rightarrow CO_2 + 1/2 N_2$ on ZnO are similar to those obtained earlier for TiO₂ "Degussa". Initial rate of NO and CO photo-adsorption was shown to be linearly dependent on radiation intensity. Since spectral dependences for initial rates of C₂H₆ and NO photo-adsorption were concurrent, the conclusion about NO absorption on photo-activated hole centers with creation of NO₂⁻ transition state on the surface can be made.

References

1. Andrei A. Lisachenko, Ruslan V. Mikhailov, Lev L. Basov, Boris N. Shelimov, Michel Che //Journal of Physical Chemistry C. 2007, V.111, P.14440-14447.

Optical characterization of GaAs based heterostructures

Blinov Grigorii
griwan.sk8@gmail.com

Scientific supervisor: Prof. Dr. Agekyan V.F., Department of Solid State Physics, Faculty of Physics, Saint-Petersburg State University

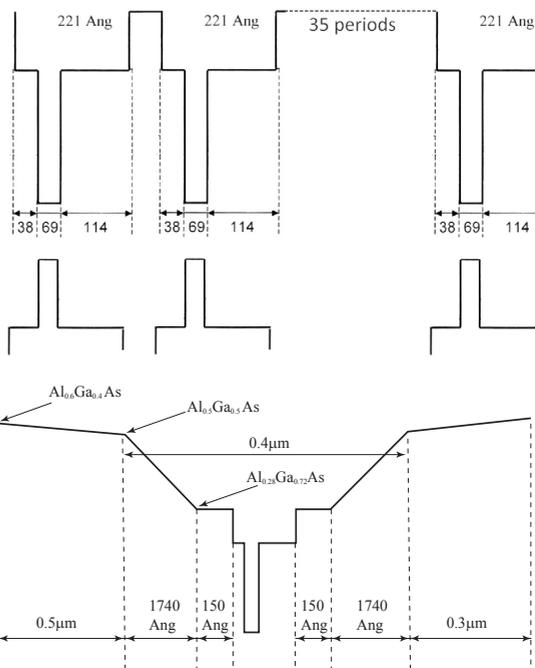
Optical properties of two GaAs based quantum well (QW) structures are studied, their energy profiles are shown at the figures. Low temperature luminescence, reflection and luminescence excitation spectra have been investigated.

The reflection spectrum of sample №1 shows the structure near 1,89 eV associated with a barrier exciton.

One can also observe a periodical interference structure in the energy range of the sample transparency. The luminescence band near 1,88 eV is considered as a barrier exciton emission. The low-energy band near 1,64 eV can be attributed to QW exciton. The luminescence excitation spectrum shows only one feature originated from a barrier exciton.

The high-energy feature near 1,89 eV associated with a barrier exciton can be seen in the reflection spectrum of sample №2 along with the periodical inference structure. Three bands are observed in the luminescence at 1,87 eV (barrier exciton), 1,67 eV and 1,62 eV. We have found only the barrier exciton structure in the luminescence excitation spectrum.

We discuss the interpretation of the optical spectra of sample №1 and №2. The component concentrations in the heterostructures under consideration are determined from the optical data. The experimental energy level positions are compared with the calculated electron energies.



Magnetic-field induced variation of energy dispersion of exciton in CdTe

Bodnar Stanislav
stasbodnar@mail.ru

Scientific supervisor: Dr. Loginov D., Department of Solid State Physics, Faculty of Physics, Saint-Petersburg State University

Variation of exciton dispersion in magnetic field was extensively studied since 2007 [1, 2]. In these studies, optical reflection spectra for a nanostructure with CdTe/CdZnTe QW in magnetic field (Voigt geometry) are discussed. It has been shown that application of magnetic field to the sample leads to the change of exciton dispersion. These changes are described in framework of the perturbation theory considering operator:

$$V = \frac{2a_b h e}{cM} K B_x I \quad (1)$$

where e is the electron charge, c is the velocity of light, M is the mass of exciton, K is the exciton wave vector, B_x is the magnetic field, h is the Planck constant, a_b is the Borh radius.

The change of exciton dispersion was explained in papers [1,2] via change of effective mass of exciton. It is calculated in the *second order* of perturbation theory using operator (1).

At the same time, in papers [3, 4] this effect was explained as non-parabolic dependence of exciton dispersion induced by magnetic field. The non-parabolic dependence is calculated using operator (1) in the *first order* of perturbation theory.

In our work, we compare contributions to the changes of exciton dispersion related to two these mechanisms. Calculation has shown that these contributions are almost of the same value.

References

1. D. Loginov, V.P. Kochereshko, A. Litvinov, L. Besombes, H. Mariette, J.J. Davies, L.C. Smith and D. Wolverson //Acta Phys. Pol. A, 112, N2, 381-386, (2007).
2. D.K. Loginov, V.P. Kochereshko, R.T. Cox, L. Besombes, H. Mariette, J.J. Davies, D. Wolverson, and L.C. Smith //Phys. Status Solidi B, 247, No. 6, 1528–1530 (2010).
3. D.K. Loginov // Physics of the Solid State, 52, No. 1, 70-78 (2010).
4. D.K. Loginov and A.D. Chegodaev // JETP, 113, No.3, 502-509 (2011).

Defects and structure study of ferromagnetic opal-like films by GISAXS technique

Dubitskiy Ilya, N.A. Grigoryeva, A.A. Mistonov, I.S. Shishkin,
S.V. Grigoriev
i.dubitsky@phys.spbu.ru

Scientific supervisor: Prof. Dr. Grigoriev S.V., Department of Nuclear Physics Research Methods, Faculty of Physics, Saint-Petersburg State University

Inverse opal-like structures (IOLS) formed by filling the structural voids of the artificial opals by the different materials have attracted much attention in recent years. In particular, IOLS made from ferromagnetic materials are of interest due to using of them as a model object to solve the fundamental problem of the frustrated magnetism in 3D ordered metamaterials [1]. First step towards the study of magnetisation distribution in IOLS films is their structural characterization. It is of importance to investigate defect types IOLS possesses since defects can affect IOLS magnetic properties significantly.

IOLS were investigated by means of grazing incidence small angle X-ray scattering (GISAXS) technique. It was revealed that GISAXS could be used only for structural characterisation of 2D and quasi 2D (0.5 - 3 layers) samples since X-ray penetrating power in metals is rather low in the GISAXS geometry.

GISAXS patterns consist of vertical stripes set. In general, these stripes can be a result of both form factor and structure factor contributions to X-ray scattering. In order to reveal their origin full GISAXS simulation was carried out in ISGISAXS package [2]. It was found out, that form factor contributes to the scattering only in the case of half layer thickness Ni IOLS since form factor fluctuation is rather low for such samples.

Simple model of X-ray scattering due to structure factor was developed and found to be in a good agreement with experimental data. Additionally AFM investigations of IOLS surfaces were provided. Periodicity (500 nm) and correlation length (several microns) were found to almost coincide with those measured by GISAXS technique.

In general it was found that main type of defects quasi 2D IOLS possess are imperfections of the first type by Guinier with rather large correlation length (up to 10 microns). Therefore these structures are suitable for further investigations of its magnetic properties.

References

1. A.A. Mistonov, N.A. Grigoryeva et al. // Physical Review B, 87 (22), 220408 (2013).
2. R. Lazzari // Journal of Applied Crystallography, 35(4), p. 406-421,(2002).

Interpretation of Raman spectrum of cyclic clusters (ZnO)_n within the polarizable bond model

Dymnikova Daria
daria.dymnikova@gmail.com

*Scientific supervisor: Prof. Dr. Smirnov M.B., Department of
Solid State Physics, Faculty of Physics, Saint-Petersburg State
University*

Raman spectroscopy in the past years often used as an important experimental tool for fast characterization of materials. It is an inelastic scattering of light with momentum and energy transfer between the photons and phonons. In first-order Raman process gives the vibrational frequencies of the scattered material by the shifts of the photon frequencies. The intensities of the Raman lines characterize the vibrational eigenmodes and dielectric response of the material. The simplicity of the experiment makes this technique one of the principal methods used in vibrational spectroscopy [1, 2].

Theoretically Raman spectrum can be obtained by direct quantum-mechanical (QM) calculation. This calculation can be very difficult and can take a lot of time, in this case one can use empiric potential calculations (for frequencies) accompanied by use of the polarizable bond (PB) model (for Raman intensities). This approach is of a special interest for studying polyatomic nanostructures. To be successful this method inevitably involves reliable estimation for model parameters. The aim of this study is to estimate these parameters for the ZnO clusters, which attracted a great attention owing to perspectives for various applications [3].

References

1. A. Jorio, M.S. Dresselhaus, R. Saito, G. Dresselhaus. Raman Spectroscopy in Graphene Related Systems, John Wiley & Sons, 2011 - 368 p.
2. M. Opel and F. Venturini // European Pharmaceutical Review 7, 76 (2002).
3. X. Wang, B. Wang, L. Tang, L. Sai, J. Zhao // Physics Letters A 374 (2010) p 850–853.

Structural stability of $(\text{Ba}_{0.5}\text{Sr}_{0.5})(\text{Co}_{0.8}\text{Fe}_{0.2})_{1-x}\text{Nb}_x\text{O}_{3-\delta}$ at intermediate temperature depending on the Nb concentration

Egorova Yulia
Startjuli@gmail.com

Scientific supervisor: Prof., Dr. Filatova E.O., Department of Solid State Electronics, Faculty of Physics, Saint-Petersburg State University

$\text{Ba}_{0.5}\text{Sr}_{0.5}\text{Co}_{0.8}\text{Fe}_{0.2}\text{O}_{3-\delta}$ (BSCF) is a mixed ionic-electronic conducting (MIEC) cubic perovskite oxide (general formula $\text{ABO}_{3-\delta}$). Due to extraordinary conducting properties of BSCF combined with excellent structural and chemical stability at high temperatures it has recently attracted great attention as cathode material for solid oxide fuel cells (SOFC).

However, at low and average temperatures (800-1000°C) BSCF suffers from a slow decomposition of a cubic phase into variants with hexagonal stacking that act as barriers to oxygen transport resulting in strong reduction of the BSCF performance [1]. One of the ways to solve the problem of phase stability of BSCF at intermediate temperatures is to partly substitute the B-site cations by niobium (Nb^{5+}) [2]. In this work we discuss the possibility to stabilize the crystal structure of $(\text{Ba}_{0.5}\text{Sr}_{0.5})(\text{Co}_{0.8}\text{Fe}_{0.2})_{1-x}\text{Nb}_x\text{O}_{3-\delta}$ by partial substituting niobium for Co and Fe atoms.

We are focusing on the study of structures with different content of Nb substitution to establish the amount of the Nb, which allows us to stabilize the crystal structure of BSCF at intermediate temperatures. All the studies were carried out using near edge X-ray absorption fine structure (NEXAFS) technique. It was established that only in the 10% Nb substituted BSCF samples Co atoms occur in oxidation state close to the Co^{2+} oxidation state and is characterized by presumably octahedral symmetry of the nearest environment atoms that allows phase stabilization. In all other structures Co atoms are in $\text{Co}^{3+}/\text{Co}^{2+}$ oxidation state and occupy both octahedrally and tetrahedrally coordinated sites. Obtained results indicate the fact that for all the investigated Nb substituted BSCF systems the most optimal conditions for cubic phase stabilization at low and average temperatures are realized in the BSCF sample with 10% of Nb.

References

1. K. Efimov, Q. Xu, A. Feldhoff // Chem. Mater. 22, 5866–5875 (2010).
2. S.M. Fang, C.-Y. Yoo, H.J.M. Bouwmeester // Solid State Ionics 195, 1–6 (2011).

Synthesis and the electronic structure of graphene on the cobalt surface

Erofeevskaya Anna
anna.erofeevskaya@gmail.com

Scientific supervisor: Dr. Usachov D.Yu., Department of Solid State Electronics, Faculty of Physics, Saint-Petersburg State University

Unique properties of graphene make it perspective material for application in different technical fields and attract attention of many researchers in physics of nanostructures. For example due to large spin diffusion length [1] graphene could be used in spintronics [2]. Using graphene in any electronic devices inevitably induces graphene-metal contact and it can greatly affect the electronic properties of graphene [3]. Thus exploration of the properties of graphene synthesized on metal surfaces is an important issue. Significant interest attracts graphene/cobalt contact since cobalt is a ferromagnetic metal and could be a source of spin-polarized currents in spintronics devices.

In this work strictly oriented graphene was synthesized on monocrystalline surface of cobalt Co(0001) and electronic structure of this system was investigated. As a result dependence of crystalline and electronic structure from synthesis conditions was determined. It was found that in the case of strictly oriented graphene there is a Dirac cone near the Fermi level in the electronic structure. This cone is formed by electronic states with one spin direction localized at the graphene-cobalt interface. Moreover the mechanism of formation of spin-polarized Dirac cone in electronic structure of graphene-cobalt contact was found out. It makes a strong case for using this system for generation and control of spin current, particularly in a spin filter.

This work was supported by a grant of St. Petersburg State University No. 11.37.634.2013.

References

1. Han W. et al. // Appl. Phys. Lett. 2009.
2. Cho Y. et al. // J Phys. Chem. C 2011, 115, 6019-6023.
3. Rybkina A. et al. // Nanotechnology, 2013.

NEXAFS study of mixed ionic electronic conducting perovskite Sr(Fe,Ti)O₃

Galdina Kristina, Egorova Yulia
kris-galdina@mail.ru

Scientific supervisor: Prof. Dr. Filatova E.O., Department of Solid State Electronics, Faculty of Physics, Saint-Petersburg State University

Solid oxide fuel cells (SOFC) are electrochemical devices unlike systems based on fuel combustion. SOFCs are a promising alternative to traditional mobile and stationary power sources due to their opportunity to efficiently convert chemical energy to electricity in a silent and environmentally friendly way. Oxides with perovskite structure are compounds with chemical formula ABO₃. This is infinite origin for development of new materials with opportunity of broad-variation of their functional properties, due to crystal structure and ability to isomorphic replace in positions A and B.

The mixed electronic ionic conducting (MIEC) perovskites SrFeO₃ (SFO) and SrTiO₃ are in the focus of interest due to their possible application as membranes for oxygen separation and for solid oxide fuel cells. However, at intermediate temperatures SFO suffers from a slow decomposition and transition to an ordered brownmillerite phase (Sr₂Fe₂O₃). Also for high oxygen conductivity a high concentration of oxygen vacancies is favorable, because oxygen vacancies play a decisive role in the transport of oxygen through perovskite lattice. Substitution of Fe in SrFeO₃ with higher-valence cation Ti⁴⁺ can improve the structural stability in reducing environments. On the other hand, substitution of Fe with higher-valence Ti will decrease the oxygen-vacancy concentration in the lattice by changing the charge compensation. The optimum with respect to structural stability and oxygen conductivity may therefore be obtained by the variation of the Fe/Ti ratio in the lattice. The substitution of B-site elements will result in local distortion of the lattice and in variation of the bond length. The goal of the current work is a study of the local structure of Sr(Ti_xFe_{1-x})O_{3-δ} with purpose to analyze the structure at different Fe/Ti atoms ratio focusing on the need to stabilize the structure, while maintaining its high conductivity.

Formation of Mn/Si interface and its magnetic properties

Grebenyuk Georgy
georgijmail@gmail.com

Scientific supervisor: Dr. Pronin I.I., Laboratory of Physics of Elementary Structures of Surface, Division of Plasma Physics, Atomic Physics and Astrophysics, Ioffe Physical Technical Institute

Thin films of manganese silicide grown on a silicon surface proved of considerable interest for scientists occupied in spintronics research. Their application to development of magnetic structures requires, however, detailed knowledge of the interaction of Mn atoms with the silicon surface as well as of the reactions occurring in the Mn/Si system at elevated temperatures. The goal of the present work was to study the evolution of phase composition, electronic structure, and magnetic behavior of the Mn/Si interface *in situ* during the deposition and annealing of ultrathin metal films on the most important Si surfaces – Si(100)2×1 and Si(111)7×7.

The experiments performed in conditions of ultrahigh vacuum (10^{-10} mbar) were carried out using the Russian–German beamline of the synchrotron radiation at the HZB Bessy II electron storage ring. The elemental and chemical compositions of the silicides were studied by high-resolution photoelectron spectroscopy. This was done by measuring the series of spectra of silicon (Si 2p) and manganese (Mn 3p) core electrons, as well as of valence band electrons which were excited by 130 eV photons. The magnetic properties of interface structures were analyzed by magnetic linear dichroism in Mn 3p core-level photoemission.

It has been shown that the interfacial manganese silicide and the film of the solid solution of silicon in manganese are sequentially formed on the silicon surfaces. The growth of the metal manganese film starts after the deposition of ~0.9 nm of Mn. Segregation of silicon on the film surface is observed in the range of coverages up to 1.6 nm of Mn. After the samples annealing at different temperatures a solid solution of silicon in manganese, metallic manganese monosilicide MnSi, and semiconductor silicide MnSi_{1,7} are successively formed on the silicon surface. The films of both silicides are not continuous. The in-plane ferromagnetic ordering of the Mn/Si interface has a threshold nature and arises after the deposition of ~0.7 nm of Mn. At this coverage the ultrathin nonmagnetic layer of interfacial silicide becomes covered by a continuous film of a Si solid solution in manganese. Annealing of the film leads to the disappearance of the ferromagnetic ordering of the films at temperatures ~200°C.

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

Direct numerical solution of Schrödinger equation for excitons in quantum wells

Khramtsov Evgeniy, Belov Pavel, Grigoryev Philipp
xes2608@mail.ru

Scientific supervisor: Prof. Dr. Verbin S.Yu., Department of Solid State Physics, Faculty of Physics, Saint Petersburg State University, Spin-Optic Laboratory

One of the relevant problems in the investigation of nanostructures is to study the states of an exciton in a quantum well (QW). Analytical solution of the Schrödinger equation for this system is feasible only in particular cases [1]. Conventional approach treats the Coulomb potential as a perturbation to the size-quantized electron and hole states in a QW. We solved this problem numerically as a whole. Evaluation of the precision of the solution is important for any computational problem. Our report is aimed at such evaluation for the problem of the exciton in a QW of several exciton Bohr radius and lower.

We consider the six dimensional Schrödinger equation for electron and hole, including both the square QW potential with finite barriers' height and the Coulomb potential forming the exciton. Once we detach the analytical part of wave function (using the symmetry of the problem), we arrive to the three dimensional differential equation. Applying the finite difference method and spline decomposition method we compose a matrix, corresponding to the equation. The lowest eigenvalue of the matrix corresponds to the exciton ground state energy in QW. We use the 3- and 5-point schemes for approximation of the derivatives, that defines the precision of order of h^2 and h^4 , respectively, where h is the grid step. The spline decomposition method at equidistant grid guarantees the h^4 precision. Varying the domain width and the grid step we compare the exciton energies for a number of QW widths, and estimate the precision of various methods based on a convergence of the energy values.

Energies of the exciton ground state for various QW widths are obtained as a result of our study. Wave functions, corresponding to these energies, are compared for various methods. Excited exciton states are also obtained in the calculation. Results for QWs of width larger 30 nm (for GaAs-like semiconductor) are in good agreement against each other.

References

1. J.H. Davies, The Physics of Low-Dimensional Semiconductors, (Cambridge: Cambridge University Press, 1998), p.143.

Asymmetric Thermal Lineshape Broadening in the Dimerised Antiferromagnet $\text{BaCu}_2\text{V}_2\text{O}_8$

Klyushina Ekaterina
ekaterina.klyushina@helmholtz-berlin.de

Scientific supervisors: Prof. Dr. Bella Lake, Department Quantum Phenomena in Novel Materials, Helmholtz-Zentrum Berlin

In the conventional picture, magnetic excitations are long-lived at low temperatures with decreasing lifetime as temperature is increased. The accepted explanation is that thermally activated excitations collide with each other limiting their lifetimes -an effect observed experimentally as a Lorentzian energy broadening of the lineshape. This picture works well for gapless magnets with long-range magnetic order [1]. However for the magnets, where there are strong interactions between the excitations and the phase space is limited, this reasoning may not apply. Gapped antiferromagnets such as dimer systems which have a singlet ground state and a band of triplet excitations are potential candidates.

In present work we introduce our recent investigations of a highly dimerised 1D antiferromagnet $\text{BaCu}_2\text{V}_2\text{O}_8$ which is a potential candidate for the observation of asymmetric thermal line shape broadening. Indeed, $\text{BaCu}_2\text{V}_2\text{O}_8$ has tetragonal symmetry I-42d, where the magnetic Cu^{2+} ions (spin-1/2) form alternating spiral chains along the c-axis. Our inelastic neutron scattering measurements on a single crystal of $\text{BaCu}_2\text{V}_2\text{O}_8$ reveal that the magnetic excitations consist of two excitation branches which have a gap of 36meV and disperse along the L direction over the energy range 36-46 meV. Both modes are dispersionless in the H and K directions implying that the dimers are coupled together one-dimensionally along the c-direction, but with negligible coupling within the a-b plane. The high ratio of gap to bandwidth (=3.6) in $\text{BaCu}_2\text{V}_2\text{O}_8$ make this a candidate compound for detailed observation for asymmetric thermal lineshape broadening over a wide temperature range. In order to explore the temperature dependence of the line shape of the magnetic excitations we perform the energy scans at the dispersion minima at different temperatures. The data were fitted well by an asymmetric Lorentzian function [2] and the extracted fit parameters suggest that the line shape becomes increasingly asymmetry with increasing temperature. The results are in agreement with the recently explored temperature dependence of the magnetic excitation spectrum of copper nitrate, which is a spin-1/2 alternating chain with a similar ratio of gap to band width (=3.5) [3].

References

1. S.P. Bayrakci et al. // Science v.312, p. 1926-1929 (2006).
2. D.L. Quintero-Castro, B. Lake et al. // Phys. Rev. Lett. V.109, p. 272069 (2012).
3. D. Tennant, B. Lake et al. // Phys. Rev. B v.85, p. 014402 (2012).

Chemical bonding of organo-silicate glasses

Konashuk Aleksei
leshook@yandex.ru

Scientific supervisor: Prof. Dr. Filatova E.O., Department of Solid State Electronics, Faculty of Physics, Saint-Petersburg State University

The organosilicate glass (OSG) is nanocomposite material with peculiar physical properties due to presence of organic $-\text{CH}_3$ groups in the structure that makes OSG promising low-k dielectric with extremely low value of dielectric permittivity ($k < 2.5$) for improvement in the advanced interconnect technology. Reduction of permittivity is achieved in general both due introduction of hydrophobic organic $-\text{CH}_3$ groups and formation of low polarizable $\text{Si}-\text{CH}_3$ bonds and creating of porosity in SiO_2 -like matrix by introduction and subsequent removal of sacrificial organic porogen or by self-assembling film growth without applying the porogen.

Although it is possible to obtain quite low values of permittivity there is no clear understanding of mechanism of permittivity reduction at the level of chemical bonding and atomic electronic structure. In this connection we provide study of relation between static dielectric permittivity and atomic electronic properties of OSG using near edge X-ray absorption fine structure which is very sensitive to the nature of the absorbing atoms, their chemical state and local coordination environment. We are focusing on the study of the formation, self-organization and properties of porous OSG films with different permittivity values and synthesized using different methods with purpose to establish the factors, which are responsible for permittivity and allow reduce its value. We have established that formation of low polarizable $\text{Si}-\text{CH}_3$ bonds and introduction of porosity are two coexisting competing processes which are responsible for permittivity decreasing; main role in reducing of permittivity from 2.5 to 2.3 belongs to $\text{Si}-\text{CH}_3$ bonds and their concentration in structure. Further reduction (to 2.2 - 1.8) occurs by increasing the porosity of structure.

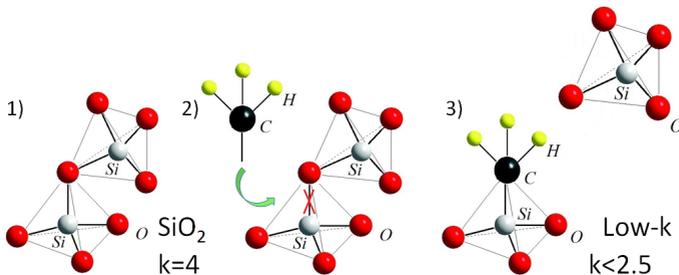


Fig. 1. Schematic representation of structure of organo-silicate glass.

X-ray spectroscopic study of oxygen scavenging from γ - Al_2O_3 -film depending on material of top electrode and its annealing

Konyushenko Marina, Konashuk Aleksei
marinakony@yandex.ru

Scientific supervisor: Prof. Dr. Filatova E.O., Department of Solid State Electronics, Faculty of Physics, Saint-Petersburg State University

Recently significant effort is directed to the study of high- k dielectric and metal gates for flash memory devices. For this application, dielectrics with large band gap (>6 eV) and band offsets, intermediate k -values (9-20) and low trap densities are required [1]. Al_2O_3 has been considered as one of the main candidate due to i) a thermodynamic stability; ii) a k -value of ~ 9 ; iii) upon crystallization, the band gap and band offsets of Al_2O_3 increases dramatically; iv) a band gap and a trap density can be controlled by the technique deposition and thermal annealing conditions. The interfacial properties of the Al_2O_3 are important in determining the height of the energy barrier for electrons at metal/insulator interfaces, which direct impact on the functionality of the flash devices [1], are of a special interest and under debate up to now.

In view of the foregoing the goal of this work was a study of electrode/ Al_2O_3 interface depending on the electrode material (TiN, TaN) and electrode's annealing to evaluate the possible oxygen scavenging from the Al_2O_3 insulator. All the measurements were carried out using near-edge-x-ray absorption fine structure (NEXAFS) on the optics beamline BESSY-II of the HZB. The measurements carried through the electrodes reveal significant oxygen scavenging from the Al_2O_3 film at the interface with TiN electrode. Annealing of the TiN electrode limits the oxygen scavenging from the Al_2O_3 film reducing the concentration of vacancies at the interface. Opposed to TiN electrode the TaN electrode protects the oxygen penetration out of the film. Moreover the annealing of the TaN electrode leads to growth of the oxygen vacancy contents in the vicinity of interface with film. All the studied Al_2O_3 films exhibit the γ -phase, but in the sample with annealed TaN electrode the formation of the polycrystalline γ -phase was observed.

References

1. J.A. Kittl et. al. // Mic. Eng., 86, 1789-1795 (2009).

Embedding potential method in electronic structure and X-Ray emission bands calculations of MgO clusters

Milov Igor
milov.igor.6990@gmail.com

Scientific supervisor: Prof. Dr. Tupitsyn I.I., Department of Quantum Mechanics, Faculty of Physics, Saint-Petersburg State University

In the present work the emission X-Ray K- and L-spectra of Mg atom in MgO crystal were considered. The crystal electronic structure was calculated with the embedding potential method. In this method a finite cluster and its crystalline environment are considered instead of an infinite crystal. The influence of the environment onto the cluster is simulated with the potential which is referred to as the embedding potential. The particular embedding potential used in the present work consists of two parts, far environment and near environment. Both parts were generated as described in [1-4].

The electronic structure calculations of different size and geometry clusters in the embedding potential were carried out with both Hartree-Fock and DFT methods. The X-Ray spectra calculated in the present work are in the qualitative agreement with the experimental data. It shows, in particular, that the embedding potential correctly reproduces the influence of the infinite crystalline environment onto the cluster.

References

1. I.V. Abarenkov // Phys. Rev. B 76, 165127 (2007).
2. P.V. Sushko, I.V. Abarenkov // J. Chem. Theory Comput. 6 (4), 1323–1333 (2010).
3. I.V. Abarenkov, M.A. Boyko, P.V. Sushko // Int. J. Quantum Chem. 113, 14, 1868-1876 (2013).
4. M.A. Boyko, I.V. Abarenkov // Int. J. Quantum Chem. 113, 14, 1877-1883 (2013).

Central peak of electromagnetic radiation from corrugated graphene

Mukhamadiarov Ruslan
mruslani13@gmail.com

Scientific supervisor: Prof. Kitorov S.A., Department of Theory of Semiconductors and Dielectrics, A.F. Ioffe Physical-Technical Institute of the Russian Academy of Sciences

The recent experimental study [1] has shown that a flat geometry of graphene is unstable that leads to forming of corrugations (Fig. 1): topological defects and ripples. A presence of these inhomogeneities results in modification of the electronic spectrum and to rearrangement of the vibrational states. Nonequilibrium effects of the electron-lattice interaction in the presence of ripples were analyzed in [2]. Our aim is to study the electromagnetic radiation of the corrugated graphene in the presence of the transport electric current in the ballistic regime. Size of ripples in graphene could reach several hundreds of nanometers [3]. Also, despite of “ultra-relativistic” character of spectrum, the ratio of Fermi velocity and speed of light much is smaller than unity and we could neglect a retardation of electromagnetic radiation. All these things give us a reason to consider motion of electrons in graphene within the classical approach.

We used several models to calculate the radiation power regarding distinct aspects. At the first model, we consider features of motion of electrons through the random distribution of ripples. At the second model, we take into account the effect of gauge fields that forced electrons to undergo oscillations and thus to radiate energy. Our results could be useful in experimental observation of graphene inhomogeneities and in constructing terahertz radiation devices based on graphene.



Fig. 1. Corrugated graphene sheet.

References

1. A.H. Castro Neto, K.S. Novoselov, A.K. Geim et al. // *Reviews of Modern Physics*, v. 81, pp. 109–164 (2009).
2. Yu. A. Firsov, N. E. Firsova // arXiv:1402.0767 [cond-mat.mes-hall] (2014).
3. A. Fasolino, J.H. Los, M.I. Katsnelson // *Nature Materials*, v. 6, pp. 858 – 861 (2007).

Beyond one-electron model of X-Ray band emission: Ti metal

Nikiforov Sergey, Ovcharenko Roman
box_nikiforov_sergey@mail.ru

*Scientific supervisor: Prof. Dr. Shulakov A.S., Department of
Solid State Electronics, Faculty of Physics, Saint-Petersburg State
University*

It is very important to study electronic structure of materials by means of X-ray spectroscopy methods, because they contain very detailed information on this fundamental characteristic of substance. Density functional theory (DFT) allow to calculate a shape of X-ray emission bands (XEB), which related to one-electron partial and local density of states energy distribution (LPDOS).

In the work we calculate K, L_{2,3} and M_{2,3} XEBs of metallic titanium by DFT method in pseudopotential approach [1] and compare this spectra with experimental data. The purpose of this research is understanding the rates of the influence of single electron and multielectron processes for correct description of the XEB shapes.

Calculations conducted in single electron model show, that XEBs of metal titanium display energy distribution in partial density of s, p and d states. Theoretic shape of M_{2,3} and L₃ XEBs are almost the same, what means their independence on the spatial localization of initial states. But single electron theoretical spectra poorly coincide with experimental one being much narrower. Moreover, fine structure observed in the high-energy part of experimental spectra, are not appeared in theoretical spectra. One can improve a coincidence of XEBs by taking into account the corrections related to the energy dependent natural width of the final states due to Auger effect in valence band. High-energy peak in M_{2,3} XEBs can be explained by manifestation of multiply ionization satellite (MIS) and also can be connected with polarizational bremsstrahlung of primary beam [2]. Complicate structure of high-energy part of L₃ band also can be explained by MIS. MND scattering on core-hole does not influence significantly on single electron spectra of titanium.

Single electron model of XEB of metal titanium can be applied to interpretation of spectra expanded by consideration of the multielectron processes such as Auger decay in valence band, multiply ionization of initial states (MIS) and specific polarizational (atomic) bremsstrahlung of electron beam.

References

1. R.E. Ovcharenko, I.I. Tupitsyn, E.P. Savinov, E.N. Voloshina, Yu.S. Dedkov, and A. S. Shulakov // Journal of Experimental and Theoretical Physics, 2014. Vol. 118, № 1. P. 11-17.
2. A.В. Король, А.Г. Лялин, А.В. Соловьёв. Поляризационное тормозное излучение. – СПб: СПбГПУ, 2004. – 301 С.

Theoretical investigation of manifestations of polar optical phonons in Raman spectra of short-period strained GaN/AlN superlattices

Pankin Dmitrii
dima-pankinl@mail.ru

Scientific supervisor: Prof. Dr. Smirnov M.B., Department of Solid State Physics, Faculty of Physics, Saint-Petersburg State University

In this study, frequencies and Raman intensities of polar optical phonons in the GaN/AlN superlattices (SL) of various layer thickness were calculated in the framework of dielectric continuum (DC) model and the model of polarizable bonds. In our calculations we took into consideration the elastic strains which arise in the layers of such structures during the epitaxial growth. Magnitudes and signs of the elastic strains estimated through the stress boundary condition are found in good agreement with the experimental data [1]. Accounting for the strain effect within the DC model consists in correction of the model parameters (TO and LO phonon frequencies) by use of the deformation potentials [3].

According to our calculations, the most intense lines in the TO-frequency spectral interval comes from the transversal modes propagating in the interface plane. These are the interface and quasiconfinment phonon modes with electric field localized primarily in the GaN layer. In the LO-region the most intensive modes are interface phonon mode and quasiconfinment phonon mode, which are localized primarily in the AlN layer. These modes are polarized in the plane of the interface. Comparison of spectra calculated with and without the elastic strain correction allowed the conclusion that the inclusion of impact of the elastic strains result a frequencies shift up to 15 cm^{-1} . The shift magnitude strongly depends on the layer thicknesses ratio. The strain effect does not qualitatively changes the line intensity versus layer thicknesses dependences, but it changes the critic thickness ratio values at which the phonon modes change their character between the interface and quasiconfinment one.

References

1. R.N. Kyutt, M.P. Shcheglov, V.V. Ratnikov, M.A. Yagovkina, V.Yu. Davydov, A.N. Smirnov, M.M. Rozhavsckaya, E.E. Zavarin, and V.V. Lundin // Crystallography Reports, 2013, Vol. 58, No. 7, pp. 953–958.
2. V.Yu. Davydov. Doctor thesis (Ioffe Physical Technical Institute), 2009.
3. J.-M. Wagner, F. Bechstedt // Applied Phys. Lett. 77, 346 (2000).

Magnetic anisotropy of ultrathin Fe films on the SiO₂/Si (111) surface

Pavlov Alexander
redbullsf@yandex.ru

Scientific supervisor: Dr. Ustinov A.B., Department of Physical Electronics, Institute of Physics Nanotechnology and Telecommunications, Saint-Petersburg State Polytechnic University

Many papers have been published recently on studies of the magnetic properties of ferromagnetic thin films on semiconductors surfaces. Materials appearing in these papers are Fe / GaAs and Fe / ZnSe. However, due to the fact that silicon is the most studied and used semiconductor of contemporary electronics and iron, in turn, has a high saturation magnetization value (1700 Gs) and a high Curie temperature (1044 K), of special interest are samples of Fe on Si.

This work is dedicated to experimental measurement of the polarization of the secondary electrons emitted from the structure Fe/SiO₂/Si (111). For obtaining the films the method of Fe epitaxial growth on the surface of the single crystal SiO₂/Si (111) was used. Analysis of the spectra of secondary electron spin polarization allowed us to determine magnetic properties of the obtained films. To explain the measured magnetic properties were also investigated topology films obtained using the method of scanning tunneling microscopy.

The results were following: the deposition rate of Fe on SiO₂/Si (111) was determined by Auger-electron spectroscopy, films with thicknesses of 1.2 and 1.7 nm were produced and secondary electron polarization spectra for these films were measured for two orthogonal directions of magnetization. The data suggest the presence of magnetic anisotropy in ultrathin iron films on SiO₂ surface. This is, most probable, due to the surface anisotropy. This is confirmed by means of scanning tunneling microscopy. Taken images confirmed that there is a strong heterogeneity of the surface.

Similar studies have been performed previously using other methods (ARPES, MOKE) of research and for the other samples. However our results are consistent with these previously published papers and complement them [1,2].

References

1. S.V. Komogortsev, S.N. Varnakov, S.A. Satsuk, I.A. Yakovlev, S.G. Ovchinnikov // Journal of Magnetism and Magnetic Materials – 2014, V. 351, P. 104-108.
2. Ernst Schlömann // Journal of Applied Physics, 1970, V. 41, P. 16 - 17.

Graphene synthesis by segregation of carbon atoms through the Ni film

Pudikov Dmitrii, Zhizhin Evgeny
gelbry@gmail.com

Scientific supervisor: Prof. Dr. Shikin A.M., Department of Solid State Electronics, Faculty of Physics, Saint-Petersburg State University

The development of methods of graphene synthesis and the study of its electronic structure are the main objects of a huge number of papers in the present time due to its outstanding physicochemical properties. Unique transport properties (e.g. the highest electron mobility among all known materials) make graphene a promising material for application in different fields; in particular, it can become a basis for future nanoelectronics and a possible replacement for silicon in integrated circuit chips. The most promising applications for graphene are superfast electrical circuits, gas and photo detectors, etc.

The presence of two and more graphene monolayers strongly affects its electronic structure. Therefore one needs an appropriate synthesis method to fabricate a graphene with desired properties. The following techniques are widely used in the present time: mechanical exfoliation, thermal graphitization of silicon carbide (SiC), cracking of carbonaceous gases (CVD) and others. The main disadvantage of these methods despite their popularity in fundamental studies is the inability to use them with insulating substrates, such as SiO₂, thus making difficulties for the development and production of new devices with graphene. So the development of new methods of controllable graphene synthesis especially on insulating substrates is the most promising task in the present time.

Recent researches showed the possibility of graphene synthesis with the use of HOPG [1] or SiC as a substrate with a Ni layer atop. These systems are not metallic and the temperatures needed are rather low (<1000°C) so this technique is very attractive for creation of graphene-based devices. The aim of this work is the determination of graphene fabrication possibility by the method based on segregation of carbon atoms under the influence of heating.

References

1. X. Mingsheng, F. Daisuke, S. Keisuke, W. Eiichiro, H. Nobutaka // arXiv:1006.5085, (2010).

Synthesis of graphene by decarbidization of Gd

Shevelev Victor
victorshevelev@yandex.ru

Scientific supervisor: Prof. Dr. Vladimirov G.G., Department of Solid State Electronics, Faculty of Physics, Saint-Petersburg State University

Recently there has been increased interest in the study of graphene-based systems. This is because of the unique properties of graphene such as a linear dispersion relation, anomalously high mobility of charge carriers. The aim of this work was to study the possibility of the formation of graphene as a result of carbidization-decarbidization of the system formed on the basis of gadolinium films on the surface of HOPG. Core-level photoelectron spectroscopy and angle-resolved photoelectron spectroscopy were used for the analysis of the electronic structure. Gadolinium film was deposited on the HOPG, then the system was annealed at temperatures from 320 to 1130 °C. After annealing at $T = 745$ °C on photoemission spectra peaks are observed, which are located at $E_b = 282.9$ and 280.0 eV and shifted in energy relative to the peak of C1s HOPG. Their appearance can be attributed to the formation of gadolinium carbides - Gd_2C_3 и GdC_2 .

Increasing the annealing temperature leads to the reduction in the intensity of these peaks, indicating that decomposition of the carbides. At the same time there is a peak with $E_b = 284.9$ eV, which is a little higher than the peak of C1s HOPG ($E_b = 284.5$ eV). Such value of binding energy of C1s peak is typical for graphene. On the dispersion curves of the form π - states in point K of the Brillouin zone is nearly linear with a slight bend near the Fermi level. It also includes a small area of occupied electronic states, which can be considered as evidence of electron density transfer from gadolinium to carbon. Thus, these results show that the graphene may be formed on the surface of the gadolinium / HOPG by decarbidization of gadolinium compounds with carbon, which are occurred during annealing.

Bleaching effect in resonant reflection spectra from single GaAs/AlGaAs quantum wells

Solovev Ivan
Solivan2007@yandex.ru

*Scientific supervisor: Dr. Davydov V.G., Department of Photonics,
Faculty of Physics, Saint-Petersburg State University*

The fundamental physical limitations increasingly hinder further development of silicon microelectronics. In [1] an approach is proposed to perform logical operations optically on the base of nonlinear dynamics of an ensemble of two-level systems whose behavior is described in [2]. We investigate heterostructures with GaAs quantum wells (QW) as such systems.

It is important to study the response of QW on intense optical excitation. In this paper we present the results of studies bleaching, caused by photoinduced broadening of the resonant reflection (RR) from QW.

We have studied dependence of a resonant reflectance spectrum on monochromatic pump intensity and wavelength in the spectral range from 1.510 to 1.555 eV and have come to the following conclusions:

RR spectrum obtained in the Brewster's geometry [3] has two features associated with resonances of excitons in QW (e1HH and e1LH) and a weak feature associated with bulk excitons. Bleaching effect is resonant with excitons lines indicating the role of excitons as scattering centers. Non-resonant bleaching towards high energies (nr) is observed attributed to the formation of unbound electrons and holes, which also cause broadening of the reflection spectrum. It should be noted that radiative width remains unchanged

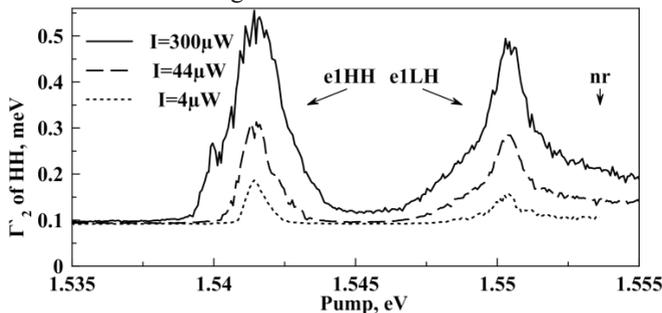


Fig. 1. Broadening (Γ_2) of RR.

References

1. Ya. Gerlovin et al. // Nanotechnology, 11, 383-386, 2000.
2. Allen L. and Eberly J. H. Optical Resonance and Two-Level Atoms, 1975.
3. S.V. Poltavtsev et al. // Sol. State Com. 199 (2014) 47-51.

Modification of the electronic and spin structure of topological insulators by noble metals intercalation

Sostina Daria
sostina37@gmail.com

Scientific supervisor: Prof. Dr. Shikin A.M., Department of Solid State Electronics, Faculty of Physics, Saint-Petersburg State University

Recently discovered materials attracted much interest in condensed matter physics. So-called three-dimensional topological insulators (TIs) belong to a class of insulators in which the bulk gap is inverted due to strong spin-orbit interaction [1-2]. A direct consequence of such a bulk band structure arises at the surface: the spin-polarized topologically protected massless metallic states form a Dirac cone. These surface states (SS) exhibit many interesting properties resulting from the fact that the spin of an electron is locked perpendicular to its momentum, forming on SS spin structure that protects electrons from backscattering. The study of the materials in question has shown them to have highly promising properties for conventional spintronics applications. Strong band bending near the surface of the prototypical TI Bi_2Se_3 was shown to lead to quantized two-dimensional electron gas (2DEG) states [3] with a very strong Rashba splitting [4], something that could be used to realize nanoscale spinfield effect transistors [5].

One of the ways to modify the electronic and spin structure is an expansion of van der Waal's spacings in layered topological TIs caused by intercalation of deposited atoms [6], leads to the simultaneous emergence of parabolic and M-shaped 2DEG bands as well as Rashba splitting of the formed states. The expansion of van der Waal's spacings and the emergence of the 2DEG states localized in the (sub)surface region are also accompanied by a relocation of the topological surface state to the lower quintuple layers, that can explain the absence of inter-band scattering.

This work is dedicated to analysis of electronic states of system, consisting of Bi_2Se_3 and materials with fractional stoichiometry such as $\text{Bi}_{2-x}\text{Te}_{2+4x}\text{Se}_{0.6}$ and $\text{Bi}_{1.5}\text{Sb}_{0.5}\text{Te}_{4.7}\text{Se}_{1.3}$ intercalated by noble metals Pt and Au. Systems were investigated by angle- and spin- resolved photoelectron spectroscopy with the application of synchrotron radiation. Experimental electronic structure and spin resolved spectra show that quantum states are spin-polarized.

References

1. Fu L. and Kane C. L. // Phys. Rev. B 76 045302, 2007.
2. Zhang H. et al. // Nature Phys. 5 438, 2009.3. Bianchi M. et al. // Nat. Commun., 1, 128, 2010.
3. King P.D. C. et al. // Phys. Rev. Lett., 107, 096802, 2011.
4. Datta S., Das B. // Phys. Lett., 56, 665, 1990.
5. Ereemeev S.V. et al. // New Journal of Physics, 14, 2012.

Study of magnetic structure of compound $\text{Mn}_{0.75}\text{Fe}_{0.25}\text{Ge}$ by small-angle neutron scattering

Sukhanov Alexander
alexander.s.sukhanov@gmail.com

Scientific supervisor: Prof. Dr. Grigoriev S.V., Department of Nuclear-Physics Research Methods, Faculty of Physics, Saint-Petersburg State University

The magnetic structure of the cubic helimagnet $\text{Mn}_{0.75}\text{Fe}_{0.25}\text{Ge}$ was studied by small-angle neutron scattering in a wide temperature range from 10 to 200 K. This compound has the cubic B20-type structure which shows the exotic spin structures appeared due to noncentrosymmetric arrangement of magnetic atoms. It is widely recognized that the helix spin structure is built on the hierarchy of interactions: ferromagnetic exchange interaction, antisymmetric Dzyaloshinskii-Moryia (DM) interaction, and the anisotropic exchange interaction [1, 2]. The ferromagnetic exchange interaction with the constant J and the DM interaction with the constant D stabilize the helix (homochiral) structure with the helix wavevector $k = D/J$. Accounting for the complex hierarchical energy scales of the system one can expect the complex magnetic phenomena upon ordering the spin structure.

In the present work was shown that $\text{Mn}_{0.75}\text{Fe}_{0.25}\text{Ge}$ has unstable helix structure below $T_N = 95$ K, since the profile of the reflection at $k = 1.7 \text{ nm}^{-1}$ associated with the spin helix can be described by the sum of Gaussian and Lorentzian contributions. The Gaussian (indicating to the stable helix) decreases with temperature while the Lorentzian (indicating to the spin helix fluctuations) increases. The spin helix fluctuations are accompanied by the intensive spin excitations detected in small angle neutron scattering as the Q -independent scattering at $Q < k$.

References

1. P. Bak, M.H. Jensen // J.Phys.C13, L881 (1980).
2. I.E. Dzyaloshinskii // Zh. Exp. Teor. Fiz. 46 1420 (1964).

Structure and Stability of WC Nanorods

Tejl Vitaliy
tejlvitalij@gmail.com

Scientific supervisor: Dr. Bandura A.V., Department of Quantum Chemistry, Institute of Chemistry, Saint-Petersburg State University

Transition metal carbides have attracted significant interest due to their unique physical and chemical properties, such as high melting point, extreme hardness, outstanding wear resistance, high bulk and Young's modulus, and high electric and heat conductivity.

In this work we present for the first time the results of ab initio calculations of the atomic and electronic structure of WC nanorods (NR) fabricated from the cubic and hexagonal phases of WC. All calculations in this work were performed by first-principles method based on density functional theory (DFT) with using of a hybrid exchange-correlation functional PBE0, as implemented in CRYSTAL09 code [1]. Spin-polarized calculations were used to estimate the effects of spin polarization. Prior to study of NR structure, the bulk and surface properties of cubic and hexagonal WC polymorphs have been examined. Obtained structural, energetic and elastic properties of both the bulk phases agree well with the available experimental and theoretical estimations. The values of surface energies calculated for thin layers parallel to (100) crystallographic planes in cubic phase and parallel to (100), (110), (101), and (001) planes in hexagonal phase are close to those obtained in recent theoretical work [2]. In accordance with experimental observations, both the bulk and nanosized forms of WC exhibit the conduction properties.

The results obtained indicate that NR stability depends on its morphology, translational axis direction, and facet indices. The lowest formation energy was found for six-facet NRs cut from the hexagonal phase along the [001] direction by {100}, {010}, and {-110} crystallographic planes. The symmetry of these NRs is described with the $P-6m2$ rod group. It was shown that the spin polarization didn't affect noticeably the atomic structure and formation energy of the considered NRs. The W and C atoms of NRs of tungsten carbide show an increase of the spin densities when moving from center of the NR to its faces. The W atoms in NRs cut from hexagonal WC phase have the largest spin densities.

References

1. R. Dovesi et al. CRYSTAL09 User's Manual, University of Torino, Torino, 2009.
2. Y. Li, Y. Gao, B. Xiao, T. Min, Z. Fan, S. Ma, D. Yi // Comput. Mater. Sci. 50, 939 (2011).

Formation and electronic structure of graphene on cobalt silicide

Vopilov Anton
antonvop@mail.ru

Scientific supervisor: Dr. Usachov D.Yu., Department of Solid State Electronics, Faculty of Physics, Saint-Petersburg State University

Graphene is a promising material for use in nanoelectronics. With a minimal thickness it demonstrates the amazing properties: high thermal conductivity, high mechanical stiffness and high mobility of charge carriers due to specific electronic structure. In the interest of a great financial and intellectual contribution to the development of silicon electronics, there is an intention to introduce graphene into existing technology. Therefore, there is significance in the study of graphene synthesized on the *metal silicide* surfaces, since they are used for making contacts in silicon devices.

The process of obtaining graphene on the surface of the cobalt silicide was studied by angle-resolved photoemission spectroscopy (ARPES). It turns out that the electronic structure of graphene on cobalt silicide is close to the electronic structure of freestanding graphene, and therefore it can be expected that this system can demonstrate many of the unique properties of graphene.

Freestanding graphene is characterized by a low concentration of charge carriers that sometimes is unprofitable. One of the effective ways to increase it is a doping of the system by alkali metal. For this purpose we have studied changes in the graphene electronic structure after adsorption of lithium atoms. The electronic structure of the resulting system was measured with ARPES, which allowed determination of the charge transfer. It turns out that the charge transfer was significantly higher than on the other substrates [1]. Thus we revealed a significant influence of the substrate on the charge transfer in graphene. High electron density allows us to expect a strong increase of the electron-phonon interaction in graphene that makes the investigated system a candidate for the detection and study of superconductivity in graphene.

This work was supported by grants of St. Petersburg State University No. 11.37.634.2013 and RFBR No. 14-02-31150.

References

1. A.V. Fedorov et. al. // Nature Commun. 5, 3257 (2014).

Features of the electronic structure of graphene on SiC with intercalated atoms of Pt

Voroshnin Vladimir
Vl.Voroshnin@yandex.ru

Scientific supervisor: Prof. Dr. Shikin A.M., Department of Solid State Electronics, Faculty of Physics, Saint-Petersburg State University

Rapid development of nanoelectronics and spintronics requires to invent new materials. Graphene, the monolayer of carbon atoms with honeycomb-like structure, is the one of the most perspective candidates. Freestanding graphene has a Dirac cone-like electronic structure near the Fermi level in the region of the K point, what determines its unique characteristics.

The electronic properties of graphene strongly depend on material of substrate, for instance graphene on Ni(111) doesn't have a linear dispersion of the pi-state, while after intercalation of one monolayer of Au underneath graphene it appears. Interaction between graphene and substrate is considered to explain this effect[1].

Moreover, corresponding spin-dependent avoided-crossing effects between the graphene pi- and metal 5d- state lead to induced spin-orbit splitting of the graphene pi-states near the Fermi level in the region of the K point. In [2] authors confirmed this statement for graphene on Pt(111). This phenomenon takes place because of hybridization between graphene pi-state and initially spin split Pt 5d states.

However, using graphene as a basic material in the nanoelectronic or spintronics requires us to synthesize it on nonconductive substrate. In this experiment we combined both important features - nonconductive substrate and spin-orbit splitting, by creating graphene on SiC(111) interface and following intercalation of atoms of Pt.

References

1. A.M. Shikin, G.V. Prudnikova, V.K. Adamchuk. // Phys. Rev. B 62, 13202–13208.
2. A.M. Shikin, A.A. Rybkina et.al. // Applied Physics Letters 105, 042407 (2014).

A complex study of copper-exchanged mordenites by XRD, XPS and ICP methods

Zhukov Yuri
yuri.m.zhukov@gmail.com

Scientific supervisor: Dr. Shelyapina M.G., Department of Nuclear-Physics Research Methods, Faculty of Physics, Saint-Petersburg State University

Composite material in which nanoparticles of transition metals are introduced into the crystal matrix, for example in the zeolite matrix, recently gained increasing use [1]. These materials have optical, electrical, magnetic properties unique between other materials. Processes for synthesizing such materials include several steps. In the case of nanomaterials deposited on the zeolite matrix those are an ion exchange reaction and the subsequent reduction reaction that leads to the formation of metal nanoparticles stabilized in a zeolite matrix. Ion-exchange zeolites are the starting materials for the synthesis of nanocomposite materials; moreover they are of great interest in themselves, because in particular transition metal, cations in zeolites are the active catalytic [2].

Recently it has been shown that the introduction of copper in the zeolite structure significantly improves the catalytic performance of the system, especially for reduction of NO_x. Though these compounds have been extensively studied in the last decade, the localization of the copper ions in the zeolite matrix and their state are not fully determined. The main difficulties are determined by the fact that the distribution of copper ions in the zeolite matrix greatly depends on various conditions including the SiO₂/Al₂O₃ molar ratio (MR) of the zeolite matrix, ion-exchange conditions, recovery processes and so on. Moreover, as a rule, these cations have high mobility and are distributed in the disordered structure of the zeolite. As a result, the localization of the cations in the zeolite matrix cannot be determined by X-ray analysis. Furthermore, the position of the copper ions depends on their valence state and of the quantity of copper ions per unit cell.

In this contribution we report on the results of our complex study by different methods (X-ray diffraction, X-ray photoemission spectroscopy, inductively coupled plasma atomic emission spectroscopy) of a series of copper-exchange mordenites with different MR and exchange degree.

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

References

1. G.D. Stucky, J.E. MacDougall // Science, 274, 669-678 (1990).
2. P. Vanelderden, J. Vacauwenberg, B.F. Sels, R.A. Schoonheydt // Coordin. Chem. Rev. 257 (2013).

F. Optics and Spectroscopy

Modeling of the argon metastable radial profile in discharge plasma

Butris Mariia
butrismasha@mail.ru

Scientific supervisor: Prof. Dr. Ionikh Y.Z., Department of Optics, Faculty of Physics, Saint-Petersburg State University

The non-equilibrium argon plasma is used in the various technological processes and gas discharge devices.

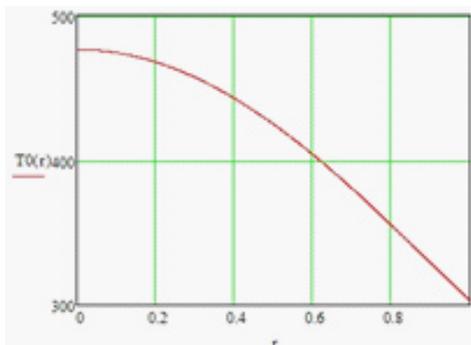


Fig. 1. The radial distribution of the gas temperature for argon discharge., $i=10$ mA, $p=40$ Torr.

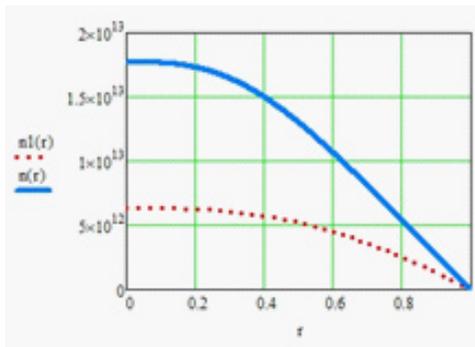


Fig.2. The $Ar(^3P_2)$ concentration when gas heating is considered (solid line) and is not considered ($T=400K$, dotted line).

In such plasmas the processes, which involve metastable atoms, play the important role in the excitation, ionization and plasma-chemistry. The metastable atoms are produced in the electron-atom collisions and de-excited at diffusion to the wall [1] and in collisions with plasma species.

It is known that diffusion rate of excited atoms depends on the gas density profile, which is affected by gas heating. Thus, the density of metastable argon atoms depends on the gas temperature profile.

In this work concentration of metastable argon atoms was calculated with considering gas heating for low-pressure gas discharge plasma [2]. In Fig. 1 the radial distribution of the gas temperature for argon at 40 Torr pressure and 10 mA current is shown. In Fig. 2 the radial profile for argon metastable 3P_2 atoms is shown with and without taking gas heating into account. It is clear that role of gas heating is very important.

References

1. Ю.З. Ионих// Оптика и спектр. 51, 76-83, (1981).
2. Y.Z. Ionikh, A.V. Meshchanov et al.// Plasma Phys.Rep., 34, 938-950, (2008).

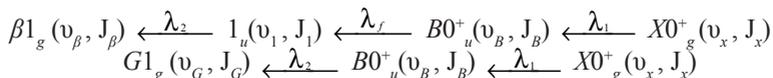
Dipole moments of the $I_2(G1_g \rightarrow 1_u(ab))$ transitions and spectroscopic characteristics of the $1_u(ab)$ states

Cherepanov Igor
cherepanov.igorfz@yandex.ru

Scientific supervisor: Prof. Dr. Pravilov A.M., Department of Photonics, Faculty of Physics, Saint-Petersburg State University

The molecule I_2 has 23 valence states correlating with three dissociation limits: (${}^2P_{3/2}$) + $I({}^2P_{3/2})$ - (aa), $I({}^2P_{3/2})$ + $I({}^2P_{1/2})$ - (ab), $I({}^2P_{1/2})$ + $I({}^2P_{1/2})$ - (bb) and 20 ion-pair (IP) states correlating with $I({}^1S)$ + $I({}^3P_J)$, $J = 2, 1, 0$, 1D , 1S , limits. Nowadays, some valence states are investigated experimentally badly. In this report I present results of study of two weakly-bound $(3,4)1_u(ab)$ states.

This work is based on the analysis of luminescence spectra from $\beta 1_g$ and $G1_g$ IP states. To populate selected rovibronic levels of IP states we successfully use stepwise two- and three-step laser excitation schemes:



The second transition in the first scheme is electric dipole forbidden in diatomic homonuclear molecules. It can be available due to hyperfine interaction between neighboring rovibronic levels of the $0_u^-(bb)$, $0_g^+(bb)$ and $1_u(ab)$ states. A detailed examination of this problem will be published in [1].

We have measured luminescence spectra from the $v_\beta = 7, 9, 17, 22, 25$ and $v_{G,0} = 6, 9$ rovibronic levels of the $\beta 1_g$ and $G1_g$ states, respectively. As a result, Dunham coefficients of the $(3)1_u(ab)$ state were determined. Besides, potential energy curve of the $(3)1_u(ab)$ and attractive limb of the $(4)1_u(ab)$ were constructed. We have determined dipole moment functions for the $I_2(G1_g \rightarrow 1_u(ab))$ transitions, also. And finally, obtained data were compared with results of accurate *ab initio* study [2]. Our spectroscopic characteristics of the $(3,4)1_u(ab)$ states are in good agreement with theoretical predictions.

References

1. Akopyan M.E., Batur V.V., Lukashov S.S., Poretsky S.A., Pravilov A.M., Vasyutinskii O.S. // J. Phys. B (2014) accepted for publication.
2. de Jong W.A., Visscher L., Nieuwpoort W.S. // J. Chem. Phys., v. 107, p. 9047 (1997).

Coherent interaction of a femtosecond laser with a dense resonant medium of atomic rubidium vapor

Elmurzaev Ruslan
elmurzaevr@bk.ru

*Scientific supervisor: Prof. Dr. Pastor A.A., Department of Optics,
Faculty of Physics, Saint-Petersburg State University*

One of the most interesting and promising problems in modern physics is the creation of a quantum computer. The study of coherent degenerate and nondegenerate four-wave processes of femtosecond pulse propagation in rubidium vapor can help in creating ultra-fast optical switches that are an indispensable part of a quantum computer.

In the article [1] a group of scientists conducted extensive experimental studies of the interaction system of broadband pulsed laser radiation and an extended optically dense two-level medium in which the phenomenon known as conical emission was observed. In the experiment, which is described in the article above, two nanosecond lasers on the solution of organic dyes were used and then excited by a pulsed Nd: YAG laser.

Investigating the interaction of coherent femtosecond laser radiation with a resonant medium of atomic rubidium vapor, we also observed the effect of conical emission and the effect of condensation on the wings of the spectrum of the resonance line. On the following diagram (Fig. 1) the change in the spectrum of the pulse passing near the resonance absorbing line can be seen, according to the temperature conditions.

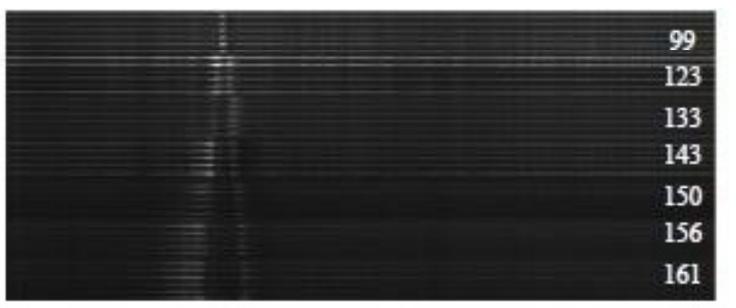


Fig. 1. Laser spectrum around the rubidium resonance line.

References

1. S.N. Bagayev, V.S. Egorov, I.B. Mekhov, P.V. Moroshkin, I.A. Chekhonin, E.M. Davliatchine, and E. Kindel // Phys. Rev. A 68, 043812 (2003).

Study of rovibrational absorption spectra of $\text{CH}_3\text{CN}\dots\text{HF}$ complexes in the gas phase

Glazachev Evgenii
eglazachev@gmail.com

Scientific supervisor: Prof. Dr. Tokhadze K.G., Department of Molecular Spectroscopy, Physical Faculty, Saint-Petersburg State University

The study of hydrogen-bonded complexes is the important area of molecular spectroscopy. The $\text{CH}_3\text{CN}\dots\text{HF}$ and $\text{HCN}\dots\text{HF}$ complexes are of interest as the model systems in the study of $\nu(\text{XH})$ band. They are amenable to a theoretical calculation and the $\nu(\text{XH})$ band has a characteristic, which allows the theoretical result to be compared with experimental data. The $\text{CH}_3\text{CN}\dots\text{HF}$ complex was studied in [1] with resolution of 2 cm^{-1} (Fig. 1-b). In present study all spectra were recorded with resolution of 0.01 cm^{-1} . The higher accuracy allows us to determine the parameters of the complex higher precision than in previous papers.

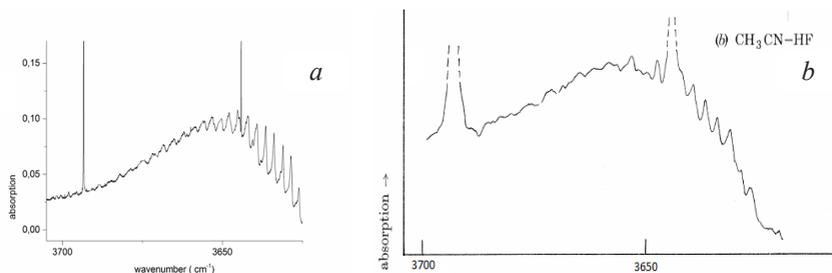


Fig. 1. Absorption spectrum of $\text{CH}_3\text{CN}\dots\text{HF}$ complex: *a* – present work, *b* – [1].

References

1. R.K. Thomas. Hydrogen Cyanide and Methyl Cyanide Hydrogen Bonding in the Gas Phase: The Infrared Spectra of Complexes of Hydrogen Fluoride with Hydrogen Cyanide and Methyl Cyanide. Proc. R. Soc. Lond. A 1971 325 October 1971.

H₂O...HF hydrogen bonded complex. Effect of H/D substitution on libration of H₂O and stretching motion of HF

Gornovesov Aleksei
gornov@bk.ru

Scientific supervisor: Prof. Dr. Tokhadze K.G., Department of Molecular Spectroscopy, Faculty of Physics, Saint-Petersburg State University

Our study is devoted to a nonempirical calculation of vibrational dynamics of the hydrogen-bonded complex H₂O...HF. Information on the structure and electro-optical parameters of such systems is obtained as a rule from spectroscopic experiments. Interpretation of experimental findings can be reliable provided that the assignment of spectral details is correct [1]. We performed a quantum-mechanical calculation of the structure, vibrational energy levels and transition frequencies of H₂O...HF and D₂O...DF. The equilibrium geometry was obtained from an *ab initio* calculation with a large set of atomic functions using the GAUSSIAN 09 package. The energy levels and vibrational transition frequencies were derived from a variational solution of the Schrödinger equation in space of librational coordinate of H₂O and stretching coordinate of HF with a very accurate nonempirical potential energy surface. Analogous calculations were also carried out for D₂O...DF. It was found that, because the barrier height of rotation of the water molecule increases with increasing HF bond length, the H-F hot transition frequency of H₂O...HF is lower than the fundamental frequency, which is at variance with the conventional point of view. Analogous results derived for D₂O...DF showed that the H/D substitution appreciably changes the relative position of fundamental and hot bands.

Reference

1. V.P. Bulychev, E.I. Gromova, and K.G. Tokhadze // Optics and Spectroscopy, Vol. 96, No. 5, pp. 774–788 (2004).

Spectral dependence of photoinduced hydrophilicity of ZnO nanofilms

Grishina Anastasia
nastasiagrishina@gmail.com

Scientific supervisor: Prof. Dr. Emelin A.V., Department of Photonics, Faculty of Physics, Saint-Petersburg State University

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 photo-induced superhydrophilicity.

To determine the hydrophilic and hydrophobic properties of the surface to make the measurement of the contact angle. If the contact angle is from 90° to 180° , such a surface is called the hydrophobic. The surface is hydrophilic, when the contact angle is from 0° to 90° . If the contact angle is less than 5° , such a surface is called superhydrophilic. Photoinduced hydrophilicity is transition to superhydrophilic state under the action of light. There are some hypotheses to explain the effect of the photoinduced superhydrophilic. That's why the aim of this work is to identify the dominant mechanism of photoinduced hydrophilicity on the films of ZnO.

At this research work ZnO films were prepared. Also kinetics of the contact angle on the surface of the original ZnO films, on the surface of films with organic substance and hydrated surface after irradiation with visible light and ultraviolet were analyzed.

Four wave mixing and computer simulation of nonlinear optical interactions

Kiselev Fedor
kisteddy@gmail.com

*Scientific supervisor: Prof. Dr. Pastor A.A. Department of Optics,
Faculty of Physics, Saint-Petersburg State University*

This paper presents the results of a computer simulation of two coupled nonlinear oscillators in the harmonic electric field and compares them with the four-wave mixing processes (FWM). Article [1] shows the calculation of processes in quasi-linear systems (or systems with low nonlinearity). This research focused on exploring our possibilities in computer simulations of optical interactions with high nonlinearity by the example of two oscillators to assess the frequency splitting of these optical processes. For numerical solution MATLAB R2013b was used. As a result we have a spectrum (Fig. 1) of this interaction with notable frequency splitting. Experiment of obtaining FWM in a polystyrene plate was performed to test the circuit and devices for further work with rubidium vapor so that we can improve our computer model and compare it with experimental data. Two pump beams of femtosecond laser strikes a point on a plane creating a diffraction grating due to thermal effects, and then third beam passes through generating fourth one.

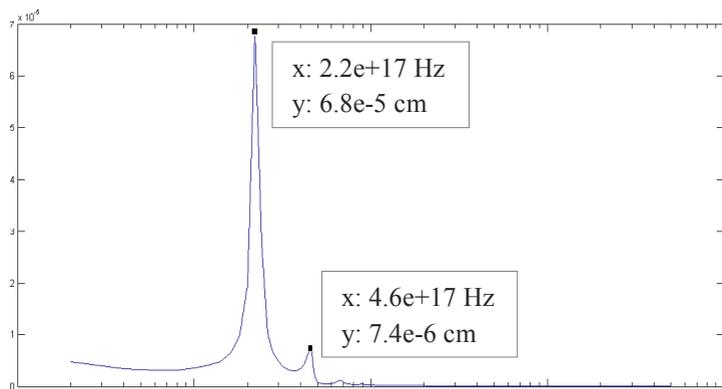


Fig. 1. Spectrum of nonlinear oscillator:

References

1. O. Kinrot, Y. Prior // Phys. Rev. A, v. 51, № 6, p. 51 (1995).

Theoretical investigation of Raman spectra of tubular ZnO nanoclusters

Kizirov Eskendir
imafreid@gmail.com

*Scientific supervisor: Prof. Dr. Smirnov M.B., Faculty of Physics,
Saint-Petersburg State University*

In present paper theoretical investigation of ZnO nanoclusters vibrational modes was performed using *ab initio* Density Functional Theory method. In this letter, we focus on study of ZnO nanoscale structures behavior for subsequent use in research on nanotubes properties. Structure optimization was performed by using of pack of quantum chemistry programs Gaussian 09.

The A^{II}B^{VI} semiconductors are technologically very important. They have been widely used in photovoltaic solar cells, optical sensitizers, quantum devices and so on [1]. The ZnO has simple crystal-growth technology, resulting in a lower cost for ZnO-based devices.

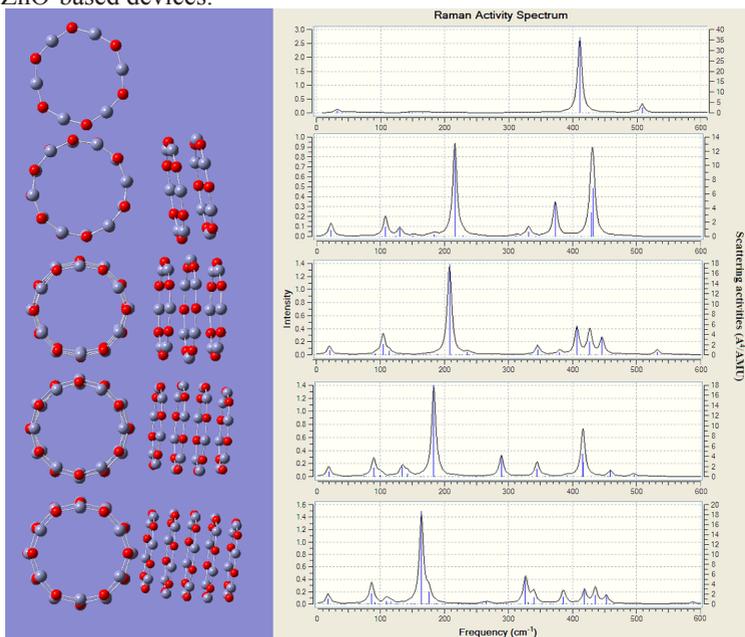


Fig. 1. Raman spectra of number of ZnO 6-molecule layers. Zn and O atoms are colored in gray and red respectively.

References

1. Chun Li, Wanlin Guo, Yong Kong, Huajian Gao // Applied Physics Letters 90, 223102 (2007).

$Y_3Al_5O_{12}:Eu^{3+}$ nanoparticles as luminescent markers for biology and medicine

Kolesnikov Ilya, D. Tolstikova, A. Povolotskiy, A. Manshina,
M. Mikhailov
ilya-kolesnikov@mail.ru

***Scientific supervisor: Prof. Dr. Pulkin S.A., Department of General
Physic I, Faculty of Physics, Saint-Petersburg State University***

Materials doped with rare-earth ions (REI) are key components of modern devices and systems for the generation, transformation and control of optical signals.

One of the most promising modern trends is the creation of nanocrystalline fluorescent particles for visualization of molecular markers in cells and tissues. The use of fluorescent labels in biology and medicine is perspective for study and characterization of lesions, diseases at the cellular and subcellular level up to the registration of individual molecules markers.

To solve the problems of medical diagnosis nanocrystalline fluorescent particles must be characterized by low toxicity, high photostability and high quantum yield, as well as possibility of surface modifying for the chemical interaction with the desired biologically active components.

The emission properties of REI-doped phosphors (stability and spectral position of luminescence) are provided by the rare-earth ion. The narrow luminescence lines and large Stokes shift allow spectral separation of excitation and emission bands and ability of simultaneous use of several labels with the independent registration. Also the possibility of REI-doped phosphors excitation in visible range can significantly increase the depth of samples diagnostic in comparison with currently used organic dyes which are typically excited by the UV radiation.

The main aim of this work is to study $Y_3Al_5O_{12}:Eu^{3+}$ nanopowders which can be considered as promising fluorescent labels for biomedical applications. The structural and luminescence properties have been investigated using various experimental techniques. The lifetime of excited Eu^{3+} level 5D_0 was measured. The possibility of detecting the luminescence signal of $Y_3Al_5O_{12}:Eu^{3+}$ nanoposphors in blood was analyzed. Also we examined luminescence time-stability of synthesized nanopowders compared with widely used organic dye – fluorescein. Finally, the ability of independent registration of nanopowders doped with different REI-ions (Eu^{3+} and Nd^{3+}) was investigated.

Acknowledgments

This work was financially supported by the Ministry of education and science of the Russian Federation (No. 14.604.21.0078). Experimental investigations were carried out in “Center for Optical and Laser Materials Research”.

Correlated librations of HCN and HF monomers in the HCN...HF hydrogen bonded complex

Koshevarnikov Alexey
koshevarnikov@bk.ru

Scientific supervisor: Dr. Bulychev V.P., Department of Molecular Spectroscopy, Faculty of Physics, Saint-Petersburg State University

In many respect the HCN...HF complex is prototypical in the studies of hydrogen bonded systems. The absorption spectra of this complex possess a resolved vibrational structure, which allows one to compare the calculated spectra with the experimental data and thereby to verify the assignment of separate spectral features. This complex was the object of extensive experimental spectroscopic studies [1]; however, its spectra have not been calculated nonempirically at a sufficiently high level of accuracy.

Our study is devoted to a quantum-mechanical calculation of simultaneous librations of HCN and HF in the complex. For this purpose, we solved the two-dimensional (2D) Schrödinger equation by the variational method using a high-precision potential energy surface computed with the GAUSSIAN package of codes. The form of potential energy surface and 2D vibrational wave functions show that the librations of monomers are strongly coupled. It was found that the 2D zero-point energy equals 348 cm⁻¹, and the frequency of transition to the first excited 2D state is 67 cm⁻¹. Judging from the shape of wave functions, this transition is associated with librational excitation of HCN. The first excited state of HF libration corresponds to the seventh 2D excited state, which gives a value of 517 cm⁻¹ for the frequency of HF libration. The results obtained are in good agreement with the experimental findings [1] and theoretical predictions [2].

References

1. D. Bender, M. Eliades, D.A. Danzeiser, M.W. Jackson, J.W. Bevan // J. Chem. Phys., v. 86, p. 1225-1234 (1987).
2. V.P. Bulychev, K.G. Tokhadze // J. Vibration Spectroscopy, v. 48, 1-9 (2014).

Spectral-luminescent study of polycrystalline phenanthrene

Kushaeva Mata
mata-kushaeva@mail.ru

Scientific supervisor: Prof. Dr. Tsyganenko A.A., Department of Photonics, Physical Faculty, Saint-Petersburg State University

Luminescence – non-thermal light emission of substance after excitement by irradiation or other factors - is widely used nowadays in life, medicine, and industry. For many purposes we are interested in the increase of the luminescence intensity. For that it is important to raise the quantum yield of the phenomenon. To this end in our work we have studied the sensibilization of luminescence by the admission of certain dopants.

Phenanthrene $C_{14}H_{10}$, is tricyclic colorless aromatic compound with melting point $99-101^{\circ}C$. First task was the study of fenantren powder. In the spectrum of luminescence four distinct bands were observed at 390, 408, 432 and 460 nm with the excitation in the range from 250 to 400 nm. The most intense in the spectrum of luminescence was the maximum at 408 nm.

The next task was a study of melted powder of fenantrene. The luminescence of such hardened sample occurs at the same spectral region, however the intensity was twice weaker as compared with the powder sample. This can be caused by some rearrangement of molecules in the structure of the sample. The positions of the bands in the luminescence spectrum did not change, but in the excitation spectrum the short-wave peak is shifted by 25 nm to the longer waves with respect to the spectrum of powder, while the long-wave peak remained at the same position.

Next task was the study of fenantrene dissolved in benzene. For the concentration of $S=10^{-2}$ mol/l the spectrum of luminescence was found to coincide in the shape and the number of bands with those of powder or fused samples, however the maxima are shifted by 5 nm to the short-wave direction. In the excitation spectrum the long-wave peak is split, while the short-wave one is absent. Besides, the intensities of both the luminescence and excitation spectra were about an order of magnitude weaker than those for the powder sample. Apparently, for the solution the spectra of individual fenantrene molecules or their conformers were detected.

To study the phenomenon of sensibilized luminescence a dopant was added to a polycrystalline sample of fenantrene. For the first essay terphenyl was chosen as a dopant. The luminescence spectra of the doped polycrystalline sample excited at 365 nm, turned out to be identical to the spectrum of the pure fenantrene matrix. Band positions are the same, but the overall intensity of luminescence is increased. We suppose that the sensitizer molecules absorb and the excitation is transferred to the matrix molecules leading to the increase of its luminescence.

Distortion of IR spectra caused by reflection

Murzin Petr, Novikov Roman
murzinpetrff@gmail.com

Scientific supervisor: Prof. Tsyganenko A.A., Department of Photonics, Faculty of Physics, Saint-Petersburg State University

Infrared spectroscopy is widely used in the studies of molecules in different states including adsorbed on solid surfaces. In these cases deviations from Lambert-Beer law could be caused by refraction at the interfaces. The present study deals with distortions in the spectra of strongly absorbing molecules, such as SF₆, CCl₄ or NF₃, in the form of films supported on transparent substrates.

Fig. 1 shows the spectrum of SF₆ deposited upon ZnSe and BaF₂ supports. The spectra are different from each other and both the bands are not symmetric and have a long “tailing” at high frequency region and sharp slope at the opposite side. Such a bandshape can be explained by reflection at the interface between the film and support. The share of reflected light varies near the absorption band, where the refraction index of the film changes greatly.

This effect was theoretically considered for liquids earlier [1, 2]. The calculated spectra are in agreement with the experimental results of present study.

The described phenomenon should be taken into account when interpreting the spectra of adsorbed molecules.

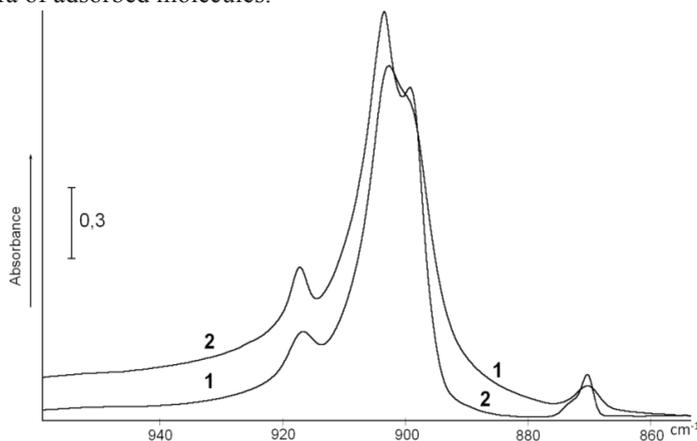


Fig. 1. Example of distortion: layer of SF₆ on: 1 – BaF₂; 2 – Si.

References

1. J.P. Hawranek, P. Neelakantan, R. P. Young, R. N. Jones // Spectrochimica Acta, Vol. 32A, pp. 85 to 98, 75 (1976).
2. R.N. Jones, D. Escolar, J.P. Hawranek, P. Neelakantan, R.P. // Young Journal of Molecular Structure, 19 (1973) 21-42.

Verification of current data and line assignments in vibro-rotational structure of the $i^3\Pi_g^{\pm} \rightarrow c^3\Pi_u^{\pm}$ band system of the H_2 molecule

Nemchaninov Alexandr, Mikhailov A.S.
aleksandr.nemchaninov@gmail.com

*Scientific supervisor: Prof. Dr. Lavrov B.P., Department of Optics,
Faculty of Physics, Saint Petersburg State University*

Diatomic hydrogen being the simplest molecule has optical spectrum, which does not have visually recognizable band structure, and looks like multiline atomic spectra. Electronic-vibro-rotational (rovibronic) spectral lines belonging to different branches, bands and band systems are located in the same spectral regions and overlap each other bringing difficulties for the line assignment. Although the first regularity within the H_2 spectrum was discovered long ago (G. Fulcher, 1913) about a half of spectral lines observed in visible part of the spectrum are not assigned or have ambiguous identification so far. Currently the book [1] represents the most complete data set for the line wavenumbers and triplet rovibronic energy levels of the H_2 molecule. Those data were obtained by traditional techniques: photographic recording of spectra and determining term values via combination differences. They were not verified by statistical analysis because this opportunity appeared only recently [2]. The optimization technique developed in [2] needs preliminary assignment of spectral lines. The assignment of lines belonging to the $i^3\Pi_g^{\pm} \rightarrow c^3\Pi_u^{\pm}$ band systems is ambiguous, because the “+”, “-“ Kronig symmetry of electronic wave functions was not included into the notation used in [1]. The goal of the present work was twofold: 1) to find a way to separate spectral lines coming to vibro-rotational levels of the $c^3\Pi_u^{\pm}$ from those coming to the levels of the $c^3\Pi_u^+$ state. 2) to prepare the data set for further statistical analysis of the wavenumbers and determination of optimal values for rovibronic energy levels by the computer code [2].

We analyzed wavenumbers of 483 spectral lines which are assigned in [1] as belonging to 57 branches of 20 bands of four different $i^3\Pi_g^{\pm} \rightarrow c^3\Pi_u^{\pm}$ electronic transitions. Constructing the Fortrat-like diagrams for experimental wavenumbers and comparing them with Rydberg-Ritz term differences made it possible to separate unambiguously 479 lines on those coming to vibro-rotational levels of the $c^3\Pi_u^{\pm}$ or the $c^3\Pi_u^+$ electronic states. For 474 lines the differences between experimental and Rydberg-Ritz wavenumber values may be characterized by the standard deviation $SD=0.15\text{ cm}^{-1}$ close to experimental error estimates, reported by G.H. Dieke.

The work was supported by the RFBR foundation (project N13-03-00786a).

References

1. The hydrogen molecule wavelength tables of Gerhard Heinrich Dieke, ed. by Crosswhite H.M. – N. Y., London, Sydney, Toronto: Wiley, 1972, - 616 pp.
2. Lavrov B.P., Ryazanov M.S. //JETP Lett. 81 (8), pp. 371-374 (2005).

Aggregation of molecules of mefenamic, niflumic and N-phenylanthranilic acid in dichloromethane solutions at various concentrations

Nosova Daria
d.kudryavceva@gmail.com

Scientific supervisor: Prof. Dr. Tsyganenko A.A., Department of General Physics 2, Faculty of Physics, Saint-Petersburg State University

Luminescence spectra of nitrogenous organic acid derivatives such as mefenamic acid, N-phenylanthranilic acid and niflumic acid in crystal phase and in solutions are known to be different [1]. To determine the impact of intermolecular interactions, we have studied the spectra of the above acids in solid phase and in the solutions in dichloromethane at different concentrations.

At concentrations less than $1.0 \cdot 10^{-4}$ mol/l the observed luminescence excitation spectra and spectra of luminescence are typical of individual acid molecules. Increasing the concentration of the solution to $1.0 \cdot 10^{-3}$ mol/l leads to formation of two types of stacking aggregates with different packing: head-to-head or head-to-tail. At this connection a splitting of the luminescence excitation spectra into two (or more) bands, shifted to higher and lower wavenumbers occurs in agreement with previously reported data [2]. The authors attributed these changes to the formation of clusters.

Since the splitting of the luminescence excitation spectrum takes place at rather low concentrations of the acids in solutions, we can talk about the spontaneous formation of aggregates and self-organization.

We can say that the concentration increase of the studied acids in dichloromethane solution leads to the formation of supramolecular structures that have their own photophysical properties. At concentrations of $1.0 \cdot 10^{-5}$ mol/l to $1.0 \cdot 10^{-2}$ mol/l is most likely the formation of J and H aggregates occurs. The maximum of luminescence of such structures appears at longer wavelengths than that of crystalline forms of the same acids.

References

1. Wang M, Zhang D, Zhang G, Zhu D // Chem. Phys. Lett. 2009,. 475. pp. 64- 67.
2. Pierola, Ines F.; Pacios, Isabel E. // J. of Fluorescence 2012,. 22 (1), pp. 145- 150.

Multiphoton ionization of rare gas from ground and metastable states

Pavlov Kirill
kirill9408@gmail.com

Scientific supervisor: Prof. Dr. Mityureva A.A., Department of Optics, Faculty of Physics, Saint-Petersburg State University

There is a growing interest in the study of multiphoton ionization of rare gases due in large part to the importance of such processes in laser physics and spectroscopy.

In our previous works [1, 2] we have performed comparison of electron- and photon-impact processes as a method for determination of photo-ionization cross sections. Using this method and values of electron-impact ionization cross sections [3, 4] we have got an absolute value of three-photon ionization cross section of ^{136}Xe from ground state:

$$\sigma_{\text{ph}}^{(3)} = 6,4 \times 10^{-83} \text{ cm}^6 \text{ s}^2$$

It is of interest to study multiphoton ionization of rare gases from excited states, especially from metastable ones. There are too few publications in this field yet [5, 6] and there is no reliable data about cross sections in such processes. But it is expected that value of cross section in such processes can be quite large. Helium is the most attractive rare gas for such investigations. We can make theoretical predictions for it, due to its simple structure.

References

1. A.A. Mityureva, A.A. Pastor, P.Yu. Serdobintsev, N.A. Timofeev // International Journal of Mathematical, Computational, Physical and Quantum Engineering Vol:7 No:11, 1043-1045(2013).
2. A.A. Mityureva, A.A. Pastor, K.V. Pavlov, P.Yu. Serdobintsev, N.A. Timofeev // Russian Journal of Physical Chemistry B (to be published).
3. R. Rejoub, B.G. Lindsay, R.F. Stebbings // Physical Review A v. 65, p. 042713 (2002).
4. K.C. Kulander // Physical Review A v. 38, n. 2, 778-787 (1988).
5. J. Bakos et al. // Sov. Phys. JETP, Vol. 44, No.2, 268-276 (1976).
6. H. Hotop et al. // Resonance ionization spectroscopy, 1992, p. 45.

NEXAFS study of composite MWCNT/(pyrolytic Cr)

Petrova Olga
teiou@mail.ru

Scientific supervisor: Prof. Sivkov V.N., Laboratory of Theoretical Physics, Mathematic Department, Komi Science Center of the Ural Division of the RAS

Coating the surface of the MWCNT specific metal coating gives them unique physical and chemical properties, and leads to the creation of new heterogeneous materials that will have good adhesion to the matrix. Such materials may be used as nanostructured heterogeneous catalysts of different chemical processes, sensors, chemical power sources, elements of various electronic devices and other active elements in the various scientific and technical applications. Therefore, the development methods of synthesis and investigations of nanostructured MWCNTs-based composite material is an actual problem. In our earlier work was demonstrated the possibility of synthesis nanosize Fe_3O_4 coating on the MWCNT surfaces by MOCVD growth technique [1] and was shown the informativity of the NEXAFS (near edge x-ray fine structure) spectroscopy for the experimental investigation of MWCNT/pyrolytic metals heterogeneous systems.

The composite MWCNT/(pyrolytic Cr) was prepared by MOCVD (Metal Organic Chemical Vapor Deposition) growth technique using as a source of chromium the mixture of bis-(benzene) Cr-metalorganic compounds which are deposited on the MWCNT surface and decomposed at temperature 400 °C with the emission of gas phase.

The NEXAFS spectroscopy allows probing the atomic composition and angular momentum character specific densities of unoccupied electronic states and may give information about chemical bonds in investigated samples. Therefore NEXAFS spectroscopy realized by the total electron yield (TEY) method can be used for studies both the thin coat and coat/substrate interface without sample destruction. In case of the composite MWCNT/(pyrolytic Cr) the coat and substrate include Cr and C atoms, respectively, that enable to study the state of MWCNT top layer and measure the Cr-coat effective thickness by the NEXAFS C1s-spectrum, and the coat chemical composition by the NEXAFS Cr2p-spectrum. But, it should be noted, that the spectral investigation of the NEXAFS C1s – edge is connected with experimental difficulties due to overlaying with NEXAFS Cr 2p – edge in the low order diffraction.

References

1. Sivkov V.N., Nekipelov S.V., Petrova O.V., Obiedkov A.M., Kaverin B.S., Kirillov A.I., Domrachev G.A., Egorov V.A., Gusev S.A., Vyalikh D.V., Molodtsov S.L. // Fullerenes, Nanotubes, and Carbon Nanostructures, 23(2015), 17-19. DOI: 10.1080/1536383X.2012.758113.

Plutonium speciation in aqueous solution studied by Pu L₃ and M₅ edge high energy resolution XANES technique

Pidchenko Ivan
ivan.pidchenko@kit.edu

Scientific supervisor: Dr. Vitova T., Institute for Nuclear Waste Disposal, Karlsruhe Institute of Technology

In this work four electrochemically aqueous plutonium (Pu) species prepared in perchloric acid solution at different oxidation states (III, IV, V, VI) as well as Pu(IV) colloids are characterized for the first time by Pu L₃ and M₅ edge high energy resolution X-ray absorption near-edge structure spectroscopy (HR-XANES). A Johann type five-analyzer crystal spectrometer recently installed and commissioned at the INE-Beamline for actinide research at the ANKA synchrotron radiation facility (Karlsruhe, Germany) was applied [1-3]. Different to conventional XANES several spectral features could be identified. The most intense absorption resonances (White Line, WL) have higher intensities for all Pu L₃ HR-XANES spectra compared to the conventional XANES. Additionally, the Pu(V) and Pu(VI) L₃ HR-XANES spectra exhibit better resolved post-edge features. The energy distance between the WL and this resonance is sensitive to the bond distance between the Pu and axial O atoms in Pu(V) and Pu(VI) [4].

Extended X-ray absorption fine structure (EXAFS) investigation is performed to correlate oxidation states with average Pu-O bonding distances. For the Pu(VI) M₅ edge HR-XANES two features at higher energy is well resolved, which might be sensitive to changes in Pu-O bond length and to the level of hybridization of metal and axial oxygen valence orbitals. The origin of hitherto unresolved features is elucidated by quantum chemical calculations using the FEFF9.5 code.

The HR-XANES experimental technique provides new insights into the actinides electronic structure and allows detection of minor contributions of Pu oxidation states in oxidation state mixtures.

References

1. J. Rothe et al. // Review of scientific instruments, 83, (2012).
2. E. Kleymenov et al. // Review of scientific instruments, 82, (2011).
3. P. Glatzel et al. // Catalysis Today, 145(3-4), (2009).
4. T. Vitova et al. // Physical Review B, 82 (23), (2010).

Excited state dynamics of substituted tetraphenylporphyrin-fullerene dyads

Pyshnyak Marina
mari-maya@bk.ru

Scientific supervisor: Dr. Povolotskiy A.V., Department of Laser Chemistry and Material Science, Institute of Chemistry, Saint-Petersburg State University

Porphyrin-fullerenes are often referred to as promising materials for artificial photosynthesis [1] and for construction of organic photovoltaic devices [2]. The electron transfer from porphyrin to the fullerene leads to the formation of the charge separated state (CS) and represents the key process in the transformation of solar energy [3]. In the development of photovoltaic devices one of the important characteristics is the lifetime of the CS state of compound.

In this work the photochemistry of tetraphenylporphyrin adducts with fullerene was studied by means of time-resolved photoluminescence and transient absorption spectroscopies upon excitation into Q-band of porphyrin. The major relaxation pathways of the singlet electronic excited state are fluorescence into the ground state (lifetime 1.3 – 8.9 ns) and intersystem crossing into the porphyrine-localized triplet excited state with lifetime of 3.6 – 7.4 μ s. The E-type delayed fluorescence originated from the porphyrin-localized triplet excited state was detected. The relatively long lived triplet CS state, which is probably originated from the porphyrine-localized triplet excited state, was revealed. We have demonstrated that the lifetime of this state depends on the substituents in the porphyrin core being up to 4 μ s for a species with *meso*-(*p*-MeOC₆H₄) substituents.

The author thanks A.S. Konev, A.F. Khlebnikov for the synthesis of compounds, A.V. Povolotskiy, A.S. Mereshchenko, Y.S. Tver'yanovich for their help in measuring UV-Vis and transient absorption nanosecond spectra, O.V. Levin for the study compounds electrochemical methods of analysis. We gratefully acknowledge the financial support of the Russian Foundation for Basic Research (Grant No. 14-03-00187) and Saint Petersburg State University (Grant No. 12.38.78.2012). A.S.M. acknowledges Saint Petersburg State University for the financial support (post-doctoral fellowship #12.50.1562.2013). Flash photolysis, luminescence and UV/VIS absorption spectra were measured at Center for Optical and Laser Materials Research, Saint-Petersburg State University.

References

1. H. Imahori // *Org. Biomol. Chem.*, 2, 1425-1433 (2004).
2. H. Imahori, T. Umeyama, K. Kurotobi, Y. Takano // *Chem. Comm.*, 48, 4032-4045 (2012).
3. N. Martin // *Chem. Comm.*, 2093-2104 (2006).

Four-wave coherent interaction of the femtosecond laser pulses with Rb vapour

Semykina Valeriya
brbrbr93@mail.ru

*Scientific supervisor: Prof. Dr. Pastor A.A., Faculty of Physics,
Saint-Petersburg State University*

This paper is devoted to research of four-wave interaction of the laser pulses with Rb vapour. This topic is extremely interesting because it is connected with one of the most promising purpose of modern physics – development of element base for optical computing.

Our laboratory learns coherent degenerate and nondegenerate four-wave mixing of the 790 nm femtosecond laser pulses with Rb vapour.

The main line of investigation is learning intensity dependence on retardation of pumping pulses.

Before entering the cell with Rb vapour the laser beam divides into three parts. Two of them arrive to the cell simultaneously, other – with time delay. We use two dielectric mirrors on quartz substrate as the divider of light radiation.



Fig. 1. The additional signals.

This paper contains excitation mechanism of the system. The system was excited from the ground state 5S to the 5D state through the intermediate 5P state. Inverted population on the 5D-6P transition produces coherent radiation with wave-length about 5 μ , which evokes radiation of visible light with 420 nm (6P-5S transition) [1]. Thus additional signals appear on the distant screen (Fig. 1). They arise because of interaction of pumping beams.

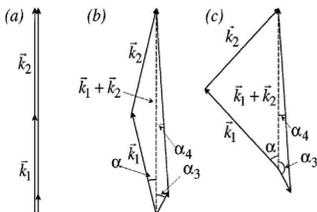


Fig. 2. Phase-matching diagram for two-pulse YSF perfluorescence in Rb

To understand why these additional signals appear, we need to resort to the phase-matching diagram for two-pulse yoked superfluorescence (YSF) in rubidium (Fig. 2).

After pumping beams pass the cell with Rb vapour they form vertexes of square, visible light with 420 nm wave-length propagates along the bisecting line generated by these beams.

Consequently conducted research confirms theoretical exposition of the four-wave mixing

References

1. A.I. Lvovsky and S.R. Hartmann // Phys. Rev., V. 82, N. 22, 1999, pp. 4420-4423.

Effect of F-doping on the photocatalytic activity of titania

Shaitanov Leonid
leoshait@yandex.ru

Scientific supervisor: Prof. Dr. Ryabchuk V.K., Department of Photonics, Faculty of Physics, Saint-Petersburg State University

Photocatalysts used in heterogeneous photocatalytic processes play an important role in different practical applications, such as air and water purification, creation of self-cleaning and bacterial coatings and other. One of the most studied photocatalysts is titanium dioxide, because of its band gap (3.0 – 3.2 eV) corresponding to UV-region of the Solar spectrum, its chemical stability and nontoxicity as well as low cost. Under the irradiation of light with energy higher than band gap, free charge carriers, electrons and holes, appear at the surface. They can be trapped by bulk and surface defects turning such defects into the chemically active state.

The main characteristic of photocatalysts is their activity. For increase of this characteristic the nonmetal doping can be used for the photocatalyst modification [1]. The introduction of the impurities can result in formation of the energy levels, within the band gap. Thus, transition of electron from these levels requires photon energy which is less than band gap energy. Accordingly, the light absorption in the visible range can appear, and, consequently, activity of photocatalyst can increase.

In our study fluorine was used as a dopant. For understanding of the processes of photoexcitation we performed experiments on the investigation of the alterations in the absorption by diffuse reflectance spectroscopy. Also kinetic parameters, such as life time and maximal rate of photoadsorption, were determined. The effect of the dopant concentration on photoinduced defect formation and activity of the surface active centers was established. The details of experimental procedures and experimental results will be discussed during presentation.

References

1. W.Y. Teoh. // *Materials*, 6 (8), pp. 3194 – 3212, 2013.

Confocal ring cavity

Shalymov Yegor
ShEV1989@yandex.ru

Scientific supervisor: Prof. Dr. Venediktov V.Yu., Laser Measurement and Navigation Department, St.-Petersburg State Electrotechnical University

Development of comparatively cheap and miniaturized (with the size of several centimeters or less) gyros for the wide range of possible applications is one of the most important tasks in the field of developing the navigation and orientation equipment. For today this area is preoccupied by various kinds of micromechanical gyros (see, for instance [1, 2]). However, these devices are sensitive to linear accelerations and to various kinds of mechanical stress, limiting thus the field of their possible applications. Optical gyros (ring laser gyros and fiber-optical gyros [3, 4]) are free of these limitations, but for various reasons their minimal diameter is limited by some 100-150 mm. Hence during the last decade the main activities in the area of developing the microoptical gyro were concentrated on the other scheme of prospective device, based on the use of passive ring single-mode cavities, which are usually produced with the use of planar integral optical technologies [5, 6].

Passive ring cavities are now treated as the most promising sensitive elements for cheap and technologically simple microoptical gyro for mass production. Usually the single-mode planar waveguides are considered to be the only possible technology for such devices implementation. However, our analysis shows that in some cases the confocal ring cavity, characterized by degeneration of transverse modes, can be the better alternative for such a device technology.

References

1. Schmidt G.T. INS/GPS Technology Trends // Advances in navigation sensors and integration technology. NATO RTO Lecture series 232, 2004.
2. Apostolyuk V. Theory and design of micromechanical vibratory gyroscopes. MEMS/NEMS Handbook, Springer, 2006, Vol.1, pp.173-195
3. Chow W.W., Gea-Banaoche J., Pedrotti L.M., Sanders V.E., Schleich W., Scully M.O. The ring laser gyro // Rev of Modern Phys. 1985, 57, 61-104.
4. Hervé Lefèvre. The Fiber-Optic Gyroscope, 1993, ARTECH HOUSE, INC.
5. Ford C., Ramberg R., Johnson K. // IEEE AES Systems Magazine, December 2000. P. 33.
6. Li G., Winick K.A., Youmans B. Design, fabrication and characterization of an integrated optic passive resonator for optical gyroscopes // ION 60th Annual Meeting, Dayton, Ohio, June 7-9, 2004.

Kerr effect and short-range order in mesogenic compound melts

Shevliagin Arsenii
arseniishevliagin@yandex.ru

*Scientific supervisor: Dr. Polushin S.G., Department of Polymers,
Faculty of Physics, Saint-Petersburg State University*

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.

References

1. Polushin S.G., Filippov S.K., Barmatov E.B., Pebalk D.A., Ryumtsev E.I. // Russ. Reports of the Academy of Sciences. V. 405. N 5, p. 634–637, (2005).
2. Rogozhin V.B., Polushin S.G., Byeloborodov I.V., Ryumtsev E.I. // Russ. J. Liquid crystals and their practical application. issue 2 (20), p. 83-91, (2007).
3. Polushin S., Rogozin V., Beloborodov I., Rjumtsev E., Kozlovsky M. // Macromolecular Rapid Communications. V.29. Issue 3, p. 224-228, (2008).
4. Goodby J.W., Petrenko A., Hird M., Lewis R.A., Meier J., Jones J.C. // Chemical Communications. p. 1149, (2000).
5. Dodge M.R., Vij J.K., Cowling S.J., Hall A.W., Goodby J.W. // Liquid Crystals. 32, p. 1045, (2005).
6. Nishiyama I., Yamamoto T., Yamamoto J., Yokoyama H., Goodby J.W. // Molecular Crystals and Liquid Crystals. 439, p. 55, (2005).
7. Cowling S.J., Hall A.W., Goodby J.W. // Liquid Crystals. 32, p.1483, (2005).
8. Polushin S.G., Rogozhin V.B., Zahryapa A.V., Ryumtsev E.I., Boiko N.I. // Russ. J. Liquid Crystals and their practical application Issue 4 (42), p. 81-85 (2012).

Adaptive optics testing at the long-distance in-door atmosphere path

Shubenkova Elena, Gorelaya Alina
elenshubenkova@yandex.ru,
gorelayaalina@mail.ru

Scientific supervisor: Prof. Dr. Venediktov V.Yu., Laser Measurement and Navigation Systems Department, Saint Petersburg Electrotechnical University "LETI"

The unique in-door atmospheric beamlet in Sosnovy Bor (Leningrad region, 80 km from St.-Petersburg) is comprised by 15 high (diffraction limited) quality 500 mm plane mirrors (HR coated for 0.53 and 1.06 micron). The maximal length of free space propagation along this beamlet is 700 m. The beamlet is placed in the capsulated compartment, placed inside the building, providing high stability and reproducibility of atmospheric conditions inside. The compartment is equipped by heaters and fans, which can provide the controlled and repeatable distortions of atmosphere inside. This test-bed provides the unique capabilities for testing various optical systems. In the past it was successfully used for various laser beam propagation studies and nonlinear-optical compensation.

In our talk we present the first results of investigations of implementation of the closed-loop adaptive optical system at the beamlet segment with the length 80-240 m. We have used the standard system of NightN Co. production (<http://www.nightn.ru/files/products/files/adsys/adsys.htm>), providing correction of not too fast (not more than 30 Hz) distortions. It was shown that under stable conditions (without heating and artificial wind) the distortions, accumulated along the path, have the magnitude of 1-2 microns (peak-to-value) and are rather slow. The use of closed-loop adaptive optical compensation in a single-mirror (flexible mirror diameter 50 mm; no tip-tilt correction) provided complete correction of these distortions down to diffraction limited performance. So our first experiments has confirmed the expectations that our beamlet can be used in future as a rather convenient test-bed for various adaptive optical systems' investigations and characterization with the rather "soft" starting conditions.

Study of the 'memory effect' at breakdown in argon-nitrogen mixture

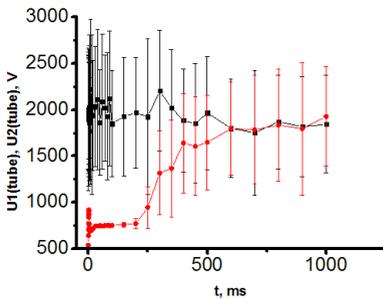
Sushentsev Danil
dan.sushentsev@gmail.com

*Scientific supervisor: Dr. Meshchanov A.V., Department of Optics,
Faculty of Physics, Saint-Petersburg State University*

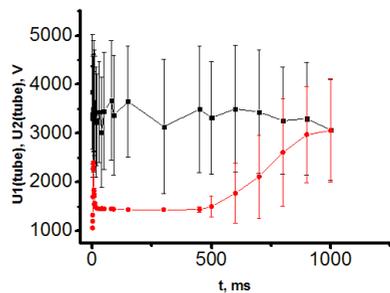
It is known from experiments that the gas discharge can influence the subsequent breakdown for some time after shutdown of the applied voltage. The influence of the previous discharge pulse on the breakdown is a subject of a number of works (see, e.g. [1]) which studied the statistical delay of the discharge pulse relative to the moment of applying the voltage to the electrodes. In those studies short discharge gaps (~ 1 mm) were investigated. To describe this phenomenon the term "memory effect of the discharge gap" was used.

The purpose of this work is to study the breakdown in a long discharge tube (75 cm) filled with argon-nitrogen (argon+0,07% nitrogen)mixture at low pressure. Similar study for the discharge in nitrogen was recently performed in [2].

In our experiment pairs of pulses were used with varied interval between the pulses of the pair. The pair repetition frequency was 0,2 or 0,5 Hz, for a gas pressure of 1 and 5 Torr. For optical measurements, we used two optical fibers connected to the PMT. The data obtained proved the existence of memory effect which was manifested as the influence of the time gap between the pulses on the breakdown voltage of the 2nd pulse. Change in pressure leads to a change in the breakdown voltage of both pulses, but does not influence existence of the effect.



1.Ar+0.07% N₂, P=1 Torr, F=0.5 Hz



2.Ar+0.07% N₂, P=5 Torr, F=0.5 Hz

References

1. M.M. Pejovic, G.S. Ristic, J.P. Karamarkovic // J.Phys. D: Appl. Phys. 35, R91-R103, (2002).
2. A.I. Shishpanov, Y.Z. Ionikh, A.V. Meshchanov, N.A. Dyatko // Plasma Phys. Rep. 40, 467-480, (2014).

Ab initio study of C—H···X hydrogen bonds along the proton transfer pathway: structure and NMR parameters

Tupikina Elena
elenatupikina@gmail.com

Scientific supervisor: Dr. Tolstoy P.M.; Center for Magnetic Resonance, Saint-Petersburg, Saint-Petersburg State University

Hydrogen bonds such as C—H···X are very prevalent non-covalent interaction in organic chemistry (in particularly, in organic molecular crystals [1] or biological structures [2]). Formation of a hydrogen bond is considered as a first step in the process of proton transfer, one of the most ubiquitous reactions in nature, $\text{CH} + \text{X} \leftrightarrow \text{C-H} \cdots \text{X} \leftrightarrow \text{C} \cdots \text{H-X}^+$.

Molecular and zwitterionic complexes in this reaction are often short-lived transient species. As a result, the structure and spectroscopic parameters remain largely unknown. In this work we considered a couple of model complexes of strong CH

proton donors with various bases (for example, a complex of 1,1-dinitroethane with pyridine, see Fig. 1). A systematic ab initio study (B3LYP/6-311++G(d,p)) of proton transfer has been carried out. We have followed changes in carbon atom hybridization along the reaction pathway, as well as NMR

spectroscopic parameters. We show that some NMR parameters (such as $^1J_{\text{CH}}$, $^1J_{\text{CC}}$, $^1J_{\text{HX}}$, $^2J_{\text{CX}}$, δ_{H}) can serve as sensitive indicators of complex's geometry. Moreover,

those theoretical results is supported by preliminary NMR experiments.

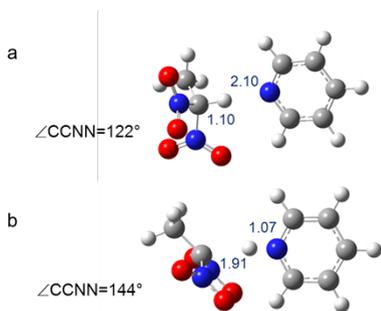


Fig. 1. Snapshots of 1,1-dinitroethane complex with pyridine: (a) equilibrium geometry, $r_{\text{CH}} = 1.10 \text{ \AA}$, (b) $r_{\text{CH}} = 1.91 \text{ \AA}$.

References

1. Desiraju G.R. // *Acc. Chem. Res.*, 24, 10, (1991) 290.
2. (a) Wahl M.C., Sundaralingam M. // *TIBS*, 22, 3, (1997) 97,
(b) Manikandan K., Ramakumar S., *Proteins*, 56, 4, (2004) 768.

Formation and researching of silver nanoparticles in phosphate glass

Vasileva Anna
111nusha111@mail.ru

Scientific supervisor: Dr. Manshina A.A., Department of Laser Chemistry and Material Science, Institute of Chemistry, Saint-Petersburg State University

Some time ago electronics was the best decision for a lot of problems but now we can see the fast development of photonics. This branch needs some new types of information storage. It is known that as an acceptable thing could be used glassy systems with transition metal. Some necessary structural modifications for creating a device can be made by femtosecond laser irradiation. We have chosen silver in phosphate matrix because of the high ability of silver to migrate in this matrix.

The aim of the research is creating silver nanoparticles in $\text{Ag}_2\text{O-P}_2\text{O}_5$ glasses with different containing of silver (from 35 to 55 mol%) by making laser induced modifications. Obtained changes were researched by optical investigation. The results of the study are could be useful for making a model of the physicochemical process which underpins investigated phenomena.

As an experiment were synthesized $\text{Ag}_2\text{O-P}_2\text{O}_5$ glasses with different containing of the silver using the melt quenching technique and after this were prepared optical transparent samples. The samples were irradiated by femtosecond Ti: Sapphire laser at 800 nm that emits 120 fs, 250 kHz pulses with 60 nJ energy. The sample was situated on 3D – translation stage. The laser beam was focused on the depth about 100 mkm from the surface. The optical research included measurement of Raman spectra (before and after laser modification) and luminescence spectra of modified zone.

After this work we have learned that laser irradiation caused global structural changes in the glass structure. Optical researching shows that silver nanoparticles were formed: there is low-frequency peak (about 84^{-1} cm) in Raman spectra after irradiation which is characteristic for silver nanoparticles. Luminescence data also confirm the assumption. Someone can see broad band in luminescence spectra at 610-650 nm. In that case we can claim that silver atoms and ions are prone to migrate in the zone of beam focus, which is the hottest. In our opinion this output is important for building the model of the nanoparticles formation process.

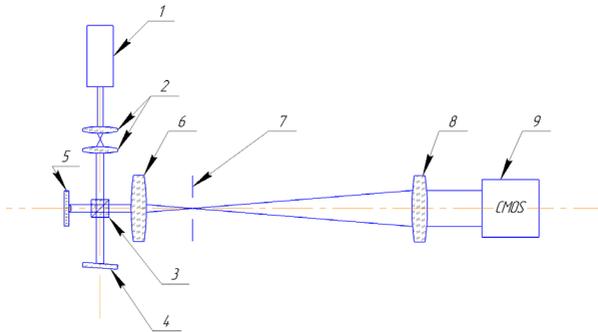
Sum up, it may be said that we realized the process of femtosecond laser induced formation of silver nanoparticles. The fact of this type of modification was proved by optical research. Some important conclusions for building a theoretical model of the process were made.

Digital holographic Michelson interferometer for nanometrology

D.V. Venediktov¹, A.A. Sevrygin¹, I.M. Tursunov¹, O.V. Volkov²
dmvened@yandex.ru

Scientific supervisor: Prof. Dr. Venediktov V.Yu., St.-Petersburg State Electrotechnical University “LETI”

1 – Saint-Petersburg State Electrotechnical Institute “LETI”
2 – St.-Petersburg National Research University of Information Technologies, Mechanics and Optics



The paper considers the dynamic holographic interferometry schemes with amplification (multiplication) of holographic fringes and with correction for distortions, imposed by the interferometer scheme elements. The use of digital microscope and of the matrix light modulator with direct addressing provides the completely digital closed-loop performance of the overall system for real-time evaluation of nano-scale objects size. Considered schemes were verified in the laboratory experiment, using the Michelson micro-interferometer, equipped by the USB-microscope and digital holography stage, equipped by the Holoeye spatial light modulator.

The method of holographic interferometry with increased sensitivity was applied for measurements of height of nano-steps (from 10 nm and higher) with standard uncertainty about 0.5 nm. The initial interferogram with equal width fringes was obtained in Michelson-type micro interferometer with nano step sample (30 μm width, 70 nm height). This interferogram was recorded by CCD-camera and the digital interference pattern was reproduced on matrix phase modulator with spatial resolution of 30 lines/mm.

The optical experiment scheme of the laser micro interferometer is shown in the figure. The described approach provides a fast and relatively simple method of magnifying interferograms.

Observation of the difference in shape of profile for lines coming to vibro-rotational levels of the $c^3\Pi_u^+$ and $c^3\Pi_u^-$ electronic states of D_2 molecule

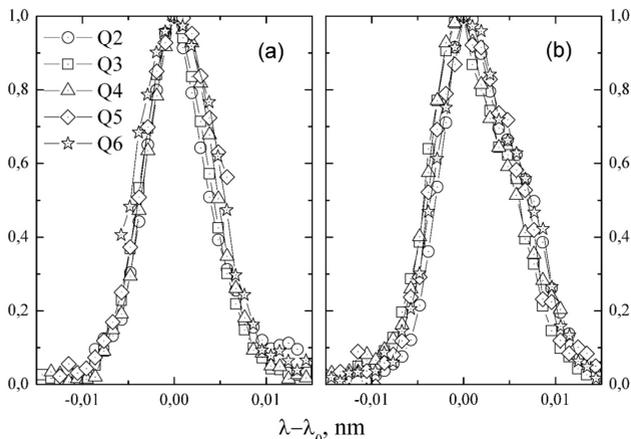
*Zhukov Alexey, Umrikhin I.S.
al.s.zhukov@yandex.ru*

***Scientific supervisor: Prof. Dr. Lavrov B.P., Department of Optics,
Faculty of Physics, Saint-Petersburg State University***

Electronic states $c^3\Pi_u^\pm$ of molecular hydrogen are important for physics of ionized gases and plasma because of extremely long lifetimes. Intensities of emission or absorption lines coming to or from the $c^3\Pi_u^\pm$ rovibronic levels may be used for spectroscopic determining their population densities. The goal of the present work was to study the line profiles in rotational structure of the $j^3\Delta_g^\pm \rightarrow c^3\Pi_u^+$ bands of the D_2 molecule.

Experimental setup was the same as in [1]. To reduce Doppler broadening of spectral lines we used constricted glow discharge with water-cooled walls under low current density (0.4 A/cm^2). We measured line profiles of the 77 pairs of spectral lines coming to identical rovibronic levels of the $c^3\Pi_u^+$ and $c^3\Pi_u^-$ electronic states. It was observed that profiles of lines coming to rotational levels of the $c^3\Pi_u^+$ and $c^3\Pi_u^-$ electronic states have noticeably different shape. As an example, the figure presents the profiles of five Q-branch lines for (0-0) bands coming from $j^3\Delta_g^\pm$ to $c^3\Pi_u^+$ (a) and to $c^3\Pi_u^-$ (b) electronic states. One may see the difference between a (symmetrical shape) and b (pseudo doublet) cases. Possible mechanisms for an interpretation of the difference are discussed.

The present work was supported by the RFBR (project N13-03-00786a).



References

1. B.P. Lavrov, I.S. Umrikhin, A.S. Zhukov //Phys.Rev. A85(5), 052505 (2012).

G. Theoretical, Mathematical and Computational Physics

Structural properties of thermoplastic polyimides in CNT-reinforced nanocomposites

Glova Artem, Serebryakov Evgenij, Larin Sergey, Lyulin Sergey
glova.temik@gmail.com

Scientific supervisor: Dr. Lyulin S.V., Laboratory №7 - Theory and Modeling of Polymer Systems, Institute of Macromolecular Compounds, Russian Academy of Sciences

Recently carbon nanotubes (CNT) attract high attention of researches due to extraordinary mechanical, electrical, and thermophysical properties. One of the promising applications of CNTs is to reinforce polymer materials to improve their physical properties. It is well known that components in composites interact mostly in the interface region. Thickness of this region and polymer matrix structure are principal parameters, which define composite properties.

In the study presented the structure of a polymer matrix in composite materials based on thermoplastic polyimides (PI) R-BAPS and R-BAPB which were synthesized and studied in the IMC RAS filled with modified CNT (m-CNT) has been studied by means of atomistic molecular-dynamics simulations. Carboxylic groups were used for the modification of the CNT surface. The influence of the surface modification degree ω on the structural properties of a composite matrix has been investigated and compared to composites filled with pristine CNT. m-CNTs with the surface modification degree $\omega = 5\%$ and 10% were considered. As have been shown recently the addition of pristine CNT to R-BAPB-based composite induces formation of layered structure in the polymer matrix that considered as a pre-crystallization stage [1]. The study of polymer density distribution relative to CNT axis shows that in composites filled with m-CNT with $\omega = 5\%$ the polymer chains can interact with m-CNT surface in contrast to composites filled with m-CNT with $\omega = 10\%$ where CNT surface is not accessible for polymer chain. However, the formation of layered structure has not observed in case of all considered composites. This behavior can be explained by effective screening of polymer interactions with CNT surface upon surface modification.

All simulations have been carried out by the computational facilities of the Institute of Macromolecular Compounds RAS, and the “Chebyshev” and “Lomonosov” supercomputers at the Moscow State University.

This study has been supported by the Russian Ministry of Education and Science within State Contract No. 14.Z50.31.0002.

References

1. S.V. Larin, S.G. Falkovich, V.M. Nazarychev, A.A. Gurtovenko, A.V. Lyulin, S.V. Lyulin // RSC Adv. 2014. V. 4. P. 830-844.

Solution of the time-dependent Dirac equation for a hydrogenlike ion exposed to a strong laser field

Ivanova Irina
ira.ivanova.v@gmail.com

Scientific supervisor: Prof. Dr. Shabaev V.M., Department of Quantum Mechanics, Faculty of Physics, Saint-Petersburg State University

Nowadays, the time-dependent problems including an interaction with intense laser fields attract much attention due to the rapid development of laser technologies. Several laser facilities operating nowadays (see, e.g., Ref. [1]) provide extremely high intensities or radiation frequencies. For instance, there is PHELIX facility (The Petawatt High-Energy Laser for Heavy Ion EXperiments) at GSI (Darmstadt). Highly charged ions are the ones of the most interesting objects that can be experimentally studied with such strong fields. FAIR (Facility for Antiproton and Ion Research, Darmstadt) will provide a unique opportunity to carry out ionization experiments with highly charged hydrogenlike ions (up to uranium) exposed to strong laser fields from PHELIX facility for testing QED effects in extremely intense fields. The theoretical description of the process under consideration is needed for such experiments at FAIR.

In present work the time-dependent Dirac equation for a highly charged hydrogenlike ion in presence of a strong laser field was solved numerically. The interaction with the intense electromagnetic pulse was considered within the dipole approximation in the length gauge. At the first stage the stationary problem in the Coulomb potential of the nucleus was solved with the dual kinetic-balance (DKB) approach [2]. At the second stage the time-dependent problem for a hydrogenlike ion in presence of a strong electromagnetic field was solved. The time-dependent Dirac wave function was expanded in terms of the stationary Dirac equation solutions. The expansion coefficients were found employing the Crank-Nicolson propagation scheme [3].

Relativistic calculations of the excitation and ionization probabilities in hydrogenlike ions exposed to strong laser fields were performed. Also convergence properties of the excitation and ionization probability values with respect to different basis set parameters used in the calculations were studied.

References

1. M. Vogel, W. Quint, G.G. Paulus, and Th. Stöhlker // Nucl. Instrum. Methods Phys. Res., Sect. B 285, 65 (2012).
2. V.M. Shabaev, I.I. Tupitsyn, V.A. Yerokhin, G. Plunien, and G. Soff // Phys. Rev. Lett. 93, 130405 (2004).
3. J. Crank and P. Nicolson // Proc. Cambridge Philos. Soc. 43, 50 (1947).

Special splints and their types

Kakin Polina
megachi@yandex.ru

Scientific supervisor: Prof. Dr. Lyakhovsky V.D., Department of High Energy and Elementary Particles Physics, Faculty of Physics, Saint-Petersburg State University

Since the term "splint" was introduced by D. Richter [1] in relation to classical root systems the attempts were made to apply it to other types of algebraic objects with varying degrees of success [2, 3]. Being a new tool of the representation theory splint allows to simplify calculation of some relations [4] while also yielding the new ones [2]. Thus generalization of splint continues to be a relevant problem.

In the present work injection fan reduction method and "special" properties of special subalgebras were used to define splint in the case of special embedding. Decomposition of the main algebra's singular element into combination of "stem's" singular elements was found and used to study properties of the new splints. Discovered special splints were studied and organized into six different types. Among them the types that allow to simplify calculation of branching rules were found. To study splints where one of the stems doesn't have the properties of a root system new definition of singular element was suggested. Together with the injection fan extension it might serve as a base for representation theory for such systems.

The type of splints where both stems don't contain the other one requires further study.

References

1. D. Richter // J. Geom. 103 (2012), pp. 103-117.
2. V.D. Lyakhovsky, A.A. Nazarov // Physics of Particles and Nuclei (September 2012), V. 43, Issue 5, pp. 676-678.
3. B. Ransingh, K.C. Pati // arXiv:1305.7189v4 (2013)
4. V.D. Lyakhovsky, A.A. Nazarov // Journal of Mathematical Sciences (New York) (2013), 192:1, pp. 91-100.

On the first order phase transitions in a large spin Fermi system

Kalagov Georgii
mygeor@yahoo.com

Scientific supervisor: Prof. Dr. Nalimov M.Yu., Department of Statistical Physics, Faculty of Physics, Saint-Petersburg State University

The equilibrium system of large spin Fermi particles (e.g. ultracold Fermi atoms with N different spin states, etc.) is studied in the formalism of temperature Green's functions

$$S = \Psi_{\alpha}^{\dagger} (\partial_{\tau} + \epsilon_p) \Psi_{\alpha} - \lambda \Psi_{\alpha}^{\dagger} \Psi_{\beta}^{\dagger} \Psi_{\beta} \Psi_{\alpha}$$

One can show [1] by the Hubbard-Stratonovich transformation at near the critical point the infrared effective action has the Landau's functional form for the complex skew-symmetric order parameter. It was shown absence infrared-stable fixed points of RG-equations for $N > 2$ by renormalization group method (three-loop calculation, MS-scheme). Methods of Borel resummation and instanton analysis (Lipatov's asymptotics) were used to study solution's behavior of RG-equations. As the result, violation of stability for Landau's functional was found. Thus the first order phase transition can occur in the system. To determine the transition temperature the RG analysis was carried out for high-order composite operators. The critical temperature for $SU(N > 2)$ system exceeds the estimates for the critical temperature of a continuous superconductive phase transition in a $SU(2)$ model, e. g. the Bardeen-Cooper-Schrieffer model.

Acknowledgement

I would like to thank M.V. Kompaniets for the cooperation.

References

1. M.V. Komarova, M.Yu. Nalimov, J. Honkonen // Theoretical and Mathematical Physics, 2013, V. 176, Issue 1, pp. 906-912.

Holographic estimates of the deconfinement temperature from the axial vector sector

Katanaeva Alisa
alice.katanaeva@gmail.com

Scientific supervisor: Prof. Dr. Afonin S.S., Department of High Energy and Elementary Particles Physics, Faculty of Physics, Saint-Petersburg State University

Holographic QCD offers new approaches to understand the strongly interacting regime of gauge theories based on AdS/CFT duality. 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 the critical temperature T_c at which hadronic matter is supposed to undergo a transition to a deconfined phase. We suppose that the influence of finite baryon density can be set to zero in the first approximation because it is negligible in the conditions of real transitions of the sort.

A rather simple method for calculating the temperature of deconfinement was proposed by Herzog [1] within the bottom-up approach to QCD, in which the deconfinement was related to a Hawking-Page phase transition between a low temperature thermal AdS space and a high temperature Schwarzschild AdS black hole.

We extend Herzog's analysis, performed for a couple of standard bottom-up models, to the soft wall model with the UV cut-off of Ref. [2]. By the way its phenomenological properties are reconsidered. In particular, we presume that this model provides a rather accurate description for the axial vector meson spectrum. The predicted value of T_c is compared with the corresponding lattice results.

References

1. Herzog C. P.// Phys. Rev. Lett., v. 98, 091601 (2007).
2. Afonin S.S.// Phys. Rev. C, v. 83, 048202 (2011).

Anomalous scaling of passive scalar fields advected by the Navier-Stokes velocity ensemble: Effects of strong compressibility and large-scale anisotropy

Kostenko Mariia
kontramot@mail.ru

Scientific supervisor: Prof. Dr. Antonov N.V., Department of High Energy and Elementary Particles Physics, Faculty of Physics, Saint Petersburg State University

The field theoretic renormalization group and the operator product expansion are applied to two models of passive scalar quantities (the density and the tracer fields) 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. The original stochastic problems are reformulated as multiplicatively renormalizable field theoretic models; the corresponding renormalization group equations possess infrared attractive fixed points. It is shown that various correlation functions of the scalar field, its powers and gradients, 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. It should be emphasized that, in contrast to Gaussian ensembles with finite correlation time, the model and the perturbation theory presented here are manifestly Galilean covariant. The validity of the one-loop approximation and comparison with Gaussian models are briefly discussed.

The results are presented in [1].

References

1. N.V. Antonov, M.M. Kostenko. Anomalous scaling of passive scalar fields advected by the Navier-Stokes velocity ensemble: Effects of strong compressibility and large-scale anisotropy, arXiv:1410.1262.

Constraint algebra for embedding theory with partial gauge fixing

Semenova Elizaveta
derenovacio@mail.ru

Scientific supervisor: Dr. Paston S.A., Department of High Energy and Elementary Particle Physics, Faculty of Physics, Saint-Petersburg State University

Research is focused on the problems related with description of gravitation. A formulation of gravitation theory in which it is supposed that space-time is 4-dimensional surface in 10-dimensional flat space is considered (first this idea was proposed by T. Regge and C. Teitelboim [1]). In this approach the function which embed the space-time into the flat 10-dimensional space is an independent variable for description of gravity [2]. Canonical formalism for embedding theory with partial gauge fixing that match time of the surface and time of the space is developed. The exact form of the first-class constraint algebra is obtained. The results obtained will be used for developing the canonical formalism for formulation of gravity as a field theory in the ambient space. In the future it may help to avoid some of the problems arising in attempts to quantize the gravity.

References

1. T. Regge, C. Teitelboim // In Proceedings of the first Marcel Grossmann Meeting, Trieste, Italy, 1975. Ed. R. Ruffini, North Holland, Amsterdam, p. 77, (1977).
2. S. Paston, A. Semenova // International Journal of Theoretical Physics, v. 49, № 11, p. 2648-2658, (2010).

Influence of radial flow fluctuations on mean transverse momentum correlations in AA collisions

Sokolskii Vladimir
sokolskiyv@gmail.com

Scientific supervisor: Dr. Altsybeev I.G., Laboratory of Ultra-High Energy Physics, Saint-Petersburg State University

Long-range correlations (LRC) between observables measured in separated rapidity intervals provide important information about the initial states of proton-proton and nucleus-nucleus collisions at high energies. The correlation strength is conventionally characterized by the correlation coefficient b_{corr} .

Different observables can be used in LRC method. In particular, correlations between mean transverse momenta of particles produced in two rapidity intervals may be considered. Such correlations arise, for example, in quark-gluon string models due to string repulsion or fusion [1].

In present report we study an appearance of mean transverse momenta correlations due to radial flow in the framework of blast-wave model [2] with the toy Monte-Carlo program. We show that event-by-event fluctuations in surface velocity of the fireball lead to this kind of correlations. It is found that correlation rises with increasing surface velocity and a magnitude of its fluctuations. It is shown also that b_{corr} are higher

for heavier particles. We conclude that the impact of radial flow should be taken into account in interpretation of the experimental measurements of mean transverse momenta correlations.

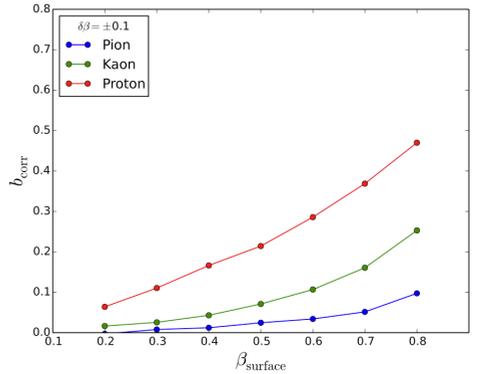


Fig. 1. b_{corr} as a function of surface velocity β , for fluctuation interval $\delta\beta=0.1$.

be taken into account in interpretation of the experimental measurements of mean transverse momenta correlations.

References

1. V.V. Vechernin and R.S. Kolevatsov // Phys.Atom.Nucl. 70 (2007) 1809-1818, Yad.Fiz. 70 (2007) 1858-1867.
2. E. Schnedermann, J. Sollfrank, U. Heinz //Phys.Rev. C48 (1993) 2462-2475; nucl-th/9307020.

Dynamics of triple asteroids

Timoshenko Vladimir
vladimir.timoshenko7@gmail.com

Scientific supervisor: Prof. Dr. Orlov V.V., Department of Celestial Mechanics, Faculty of Mathematics and Mechanics, Saint-Petersburg State University

Dynamics of several triple asteroids were studied by computer simulations and using analytical approach. We used the data of positional observations of the systems obtained by various authors [1]. Numerical results were found from initial data by integration of equations of motions in the three-body problem. We used the 4th order Runge-Kutta method with adapted step. We constructed the time dependences for osculating elements and dynamical parameters describing the system evolution. The Lidov-Kozai cycles [2, 3] were found and investigated. The stability of the systems was studied by well-known analytical criteria [4] and long-term computer experiments.

References

1. Liu X. et al. // Mon. Not. R. Astron. Soc., 2012, 427, 1034.
2. Petrovich C. // arXiv:1405.0280v1, 2014.
3. Verrier P.E., Evans N.W. // Mon. Not. R. Astron. Soc., 2009, 394, 1721.
4. Orlov V.V., Petrova A.V. // Astronomy Letters, V. 26, 2000, 250.

Sensitivity of Tunneling-Rotational Transitions in Ethylene Glycol to Variation of Electron-to-Proton Mass Ratio

Viatkina Anna
anna.viatkine@gmail.com

Scientific supervisor: Dr. Kozlov M.G., Leading Scientific Collaborator, Petersburg Nuclear Physics Institute

Ethylene glycol in its ground conformation has tunneling transition with the frequency about 7 GHz. This leads to a rather complicated tunneling-rotational spectrum. Because tunneling and rotational energies have different dependence on the electron-to-proton mass ratio μ , this spectrum is highly sensitive to the possible μ variation. We used simple 14 parameter effective Hamiltonian to calculate dimensionless sensitivity coefficients Q_{μ} of the tunneling-rotational transitions and found that they lie in the range from -17 to +18. Ethylene glycol has been detected in the interstellar medium. All this makes it one of the most sensitive probes of variation at the large space and time scales.

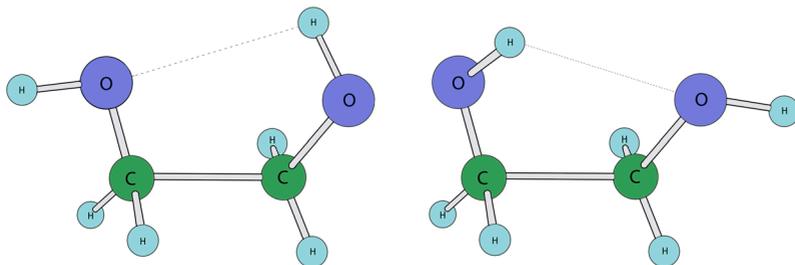


Fig. 1. Schematic molecules of ethylene glycol in two degenerate states of the conformation $g'Ga$.

H. Biophysics

Preparation of Nanoparticles by the Reduction of Silver Ions in a Solution

Dokshokova Lolita
lola.dokshokova@mail.ru

Scientific supervisor: Prof. Dr. Kasyanenko N.A., Department of Molecular Biophysics, Faculty of Physics, Saint-Petersburg State University

Over the past decade the number of publications devoted to the study of various systems containing nanoparticles of noble metals increases rapidly. Their properties significantly depend on the particle size, shape and concentration. Such systems can be useful for medicine, cosmetics, nanophotonics etc.

Nanoparticles of noble metals have unique physical, chemical and biological properties such as high electrical and thermal conductivity, chemical stability, catalytic activity, the non-linear optical behavior. The materials with nanoparticles are very attractive to use in microelectronics and medical applications. Furthermore, the silver nanoparticles have antibacterial and antifungal properties. Now the nature and strength of interactions of DNA and its components (bases and nucleosides) with metallic nanoparticles are a subject of great interest to researchers in the interdisciplines of nanobiotechnology. The first step of investigation is the fabrication of nanoparticles. We use typical procedure which base on the reduction of silver ions in a solution.

The aim of this work was the determination of the optimal conditions for the synthesis of silver nanoparticles in a solution. We tested various methods of synthesis in terms of the size of nanoparticles, their homogeneity and stability. For this study the spectral properties of the solutions were examined. We use the different ways for the reduction of Ag^+ with sodium borohydride. The optimal method for the preparation of silver nanoparticles was fined. Colloidal solutions were prepared in five different ways, and then the spectra of solutions were registered with spectrophotometer SF56 (Russia). The analysis of plasmon peak for different systems was done. We also examined the stability of the nanoparticles in solutions. The influence of DNA molecules on silver nanoparticles properties was regarded.

Excited electronic states of DNA\RNA dimers: an *ab initio* study

Maksimov Dmitry
da.maksimov.da@gmail.com

*Scientific supervisor: Kononov A.I., Department of Biophysics,
Faculty of Physics, Saint-Petersburg State University*

Excited states of nucleic acids (NAs) have been under intensive experimental and theoretical study for a long time. The interaction of DNA and RNA with ultraviolet (UV) sunlight in region above 290 nm is considered to be responsible for much photochemical damage, which leads to mutations, premature aging of the skin and carcinogenesis [1]. Although absorption spectra of NAs falls dramatically in the region above 300 nm, it is slightly overlapped with spectra of the terrestrial solar radiation, which still make them a good target for UV radiation [2].

In order to predict the electronic spectra of the nucleobase dimers and monomers we calculated vertical excitation energies and oscillator strengths at CIS level of theory. Optimized geometries of methylated monomers in ground state were obtained at HF+MP2 level using GAMESS US package. Energies of the excited states were calculated at CIS(D) and oscillator strengths at CIS level of theory as implemented in ORCA. We performed a detailed benchmark on excited energies positions depends on initial structure of monomers, using diffuse functions in basis sets and presence of solvent. Attachment and detachment of the electronic densities between ground and excited states were constructed in order to show the nature of the excitation transitions.

The low-energy transitions in all the studied structures exhibit the mostly pure exciton nature. Excitation appears to be delocalized over two bases, although a slight contribution of charge transfer between the bases to the overall state is possible. Interesting thing is that in some cases we observed rather large values of exciton splitting of monomer $\pi\pi^*$ states that come to about 0.8 eV. This value greatly exceeds the usual values 0.1 - 0.2 eV calculated for the A and B forms of homodimers [3], although the coupling strongly depends on the distance and geometry [4]. Using optimized geometries, diffuse functions and presence of solvent are also make valuable contribution to shift in red region.

References

1. Pfeifer G.P., You Y.H., Besarania A. // Mutat. Res. Fundam. Mol. Mech. Mutagen. 2005, 571, 19.
2. Sutherland J.C., Griffin K.P. // Radiat. Res. 1981, 86, 399.
3. Ritze H.H., Hobza P., Nachtigalova D. // Phys. Chem. Chem. Physics. 2007, 9, 1672.
4. Kozak C.R., Kistler K.A., Lu Z., Matsika S. // J. Phys. Chem. B. 2010, 114, 1674.

DNA Fixation on Phenanthroline-Modified Gold Substrate

Nikolaev Dmitrii, Osolodkov Mikhail
niko.dima@mail.ru

Scientific supervisor: Prof. Dr. Kasyanenko N.A., Department of Molecular Biophysics, Faculty of Physics, Saint-Petersburg State University

The fixation of DNA molecules on different surfaces is one of the problems whose solution need to conduct the appropriate researches with scanning microscopy methods, plasmon resonance method as well as to create different nanoscale structures with DNA on substrates. How to find an effective method of DNA fixation is required for different applications from AFM investigations of molecular systems to biochip technologies and other developments in such areas as genetics, proteomics, computational biology and pharmaceuticals. Usually the gold surface brings additional requirements for the attaching of biopolymers. For example, the preliminary modification of DNA molecule with specific functional groups (HS-, NH₂-) is necessary for its connection with the substrate. However, such modification is strongly hindered for long DNA strands.

In our work we use the ability of phenanthroline (Phen) molecule to bind with DNA. It is known that Phen interacts with double stranded DNA with the formation of complex with non-covalent binding (intercalation). The modification of Phen with sulfur can produce the possibility to attach Phen-SH molecule to gold surface. Such substrate can be used for DNA fixation via the intercalation of Phen into DNA helix. So the new method for the fixating of long double-stranded DNA molecules (Sigma-Aldrich Co.) on a gold substrate can be realized. Gold was chosen as the substrate material because of its conducting abilities and smooth structure, which allows studying, for example, the influence of electric fields on molecular interactions. Also the gold chips usually are the materials for the preparation of samples for the investigations with plasmon resonance method.

The investigations were performed using Plasmon 8 device (Kiev), UV-spectroscopy (SF-56, Russia), autodichrograph Mark IV (France), and low-gradient viscosimeter. DNA solutions with different concentrations of Phen-SH were used. It was shown by viscometry, that the intercalation of Phen-SH into DNA helix takes place with the saturation of binding at concentration corresponds to 1 Phen-SH molecule per 20 base pairs of DNA. The results of plasmon resonance measurements have been shown that DNA binding with the surface is observed after the modification of gold surface of chips with Phen-SH.

Electro-optical method to study aggregation in aqueous suspensions of SPIONs and SPIONs conjugated with Hsp70

Parr Marina
mparr@mail.ru

Scientific supervisor: Prof. Vojtylov V.V., Department of Molecular Biophysics, Faculty of Physics, Saint-Petersburg State University

In the present research we analyze the possibility of using electro-optical techniques to study aqueous suspensions of superparamagnetic iron oxide nanoparticles (SPIONs). Special properties of magnetic iron oxide nanoparticles open wide opportunities to apply them in medicine. Due to their superparamagnetic properties suspensions of SPIONs can be used in magnetic hyperthermia, theranostics [1], drug delivery [2] and in MRI [3]. Magnetic nanoparticles made of iron oxide possess a surface with high adsorption capacity. Due to particle aggregation aqueous suspensions of SPIONs have reduced stability. Molecules of dextran on the surface of SPIONs increase repulsion and partially stabilize the suspension. Binding of proteins to particle's surface usually increases the size of the aggregates, as the result the stability of such systems decreases. For medical applications of SPIONs we need to control the stability of the suspensions and to have rapid and robust techniques of particle aggregation analysis.

Systems of two types were prepared for electro-optical study: nonconjugated SPIONs coated with dextran and conjugates of SPIONs (also coated with dextran) with protein Hsp70. The dichroism N of the systems that was induced by the application of sinusoidal electric field was measured. For the prepared systems the relaxation curves $N(t)$ were analysed. We assessed from this experimental data for SPIONs that a considerable part of particles is not aggregated, with size 10-12 nm, but there also are aggregates with size 40-50 nm. Relaxation time of the electro-optical effect for the suspensions with conjugates increased to $5 \cdot 10^{-2}$ s, thus almost all particles in the suspension are aggregated, with aggregate size order of magnitude bigger than the size of individual particles.

The work was supported by a research grant 11.38.267.2014 of Saint-Petersburg State University.

Reference

1. K. Hayashi, M. Nakamura, W. Sakamoto, T. Yogo, H. Miki, S. Ozaki, M. Abe, T. Matsumoto, K. Ishimura // *Theranostics* V.3 (2013) 366-376.
2. P.E. Le Renard, F. Buchegger, A. Petri-Fink, F. Bosman, D. Rüfenacht, H. Hofmann, E. Doelker, O. Jordan // *Int. J. Hyperthermia* (2009) 229-39.
3. M.A. Shevtsov, L.Y. Yakovleva, et al // *Neuro-Oncology* 16(1), 2014, 38-49.

IR-investigation of DNA films

Shulenina Olga
leka-helga@yandex.ru

Scientific supervisor: Dr. Paston S.V., Department of Molecular Biophysics, Faculty of Physics, St. Petersburg State University

Alkaline metal ions and water molecules in hydrated shall of DNA molecule stabilize its secondary structure. At 100% humidity (in a solution and in a cell) B-form realizes. A-form of double helix Na-DNA can be obtained in films at 75% humidity in conditions of economical hydration of phosphate groups [1].

IR-spectroscopy is widely used for DNA structure investigations. This method allows to follow up state and nearest environment of different chemical groups of the macromolecule [2-4].

In this work water solutions of DNA and DNA films of different humidity with different content of NaCl are studied by IR spectroscopy method.

Comparison of IR-spectra of DNA samples at different humidity let us to observe influence of hydration on macromolecule structure. With growing of water content in a sample the intensity of band 1055 cm^{-1} (phosphate group's symmetrical vibrations [3-4]) descends and its form changes. In the base-sugar fingerprint region ($1250\text{-}1500\text{ cm}^{-1}$) and in the region of band 1700 cm^{-1} , assigned to in-plane double bond stretching [3-4] vibrations of bases changes of form, position and intensity are observed. At the same time band 963 cm^{-1} , which is due to sugar C-C and C-O stretching vibrations [3-4], shows high stability. That band was chosen as a normalization one.

Observed alterations in DNA IR-spectra at humidity decrease demonstrate B-A transition in the secondary structure of the macromolecule at ratios $[\text{Na}^+]/[\text{P}]$ from 1 to 66 (where $[\text{P}]$ – molar concentration of DNA phosphate groups, $[\text{Na}^+]$ – molar concentration of Na^+). However, in dependence of Na^+ content in the film the position and intensity of bands corresponding to the vibrations of phosphate groups and bases change.

Scientific research were performed at the Center for optical and laser materials research of St.Petersburg State University.

References

1. Saenger W. Principles of nucleic acid structure. – Springer Verlag, 1984.
2. Hollas J.M. Modern spectroscopy. John Wiley & Sons, Ltd.
3. Tajmir-Riahi, Naoui M., Ahmad R. // Biopolymers – 1993. – 33. – P.1819.
4. Nafisi S., Manouchehri F., Tajmir-Riahi H.A., Varavipour M. // Journal of molecular structure, – 2008. – 875. – P.392.

Estimation of photophysical parameters of silver clusters on the cytosine-containing oligonucleotide

Sych Tomash, Volkov Ivan
inxalid@gmail.com

Scientific supervisor: Dr. Kononov A.I., Department of Molecular Biophysics, Faculty of Physics, Saint-Petersburg State University

Metal clusters are a special type of nano-objects. Their main feature is that these are small in size structures consist of about ten atoms. These dimensions cause a significant contribution of quantum size effects in their electronic properties, which is why the electron-energy structure becomes similar to the molecular. The most interesting class of objects are DNA-stabilized luminescent silver clusters. They have a number of positive characteristics: significant quantum yield, high absorption cross section, good biocompatibility and photostability. All this makes them excellent candidates for use as molecular sensors and probes for the solution of bioimaging.

Photophysical parameters were investigated clusters stabilized oligonucleotide of predetermined sequence (5'-CCTCCTTCCTCC-3 '). We used methods of absorption spectroscopy, steady-state luminescence, lifetime measurement, nonlinear saturation fluorescence spectroscopy - nanosecond pulse measurements.

It is worth noting that in the course of the experiments were obtained two spectral types of clusters emitting at different bands. The first type is characterized by a spectral short-lived time (about a day) with a peak emission of ~ 630 nm, and then set a stable emission with a peak of ~ 530 nm. The second spectral type shows a steady increase over time intensity of the emission with a peak ~ 630 nm. Were received and processed by the absorption spectra of clusters of both spectral types, and the spectra of luminescence emission. By the equipment resource centers SPSU were measured lifetimes, which amounted to about 1 ns for the clusters of the first spectral type and the order of 2 ns for the clusters of the second spectral type.

In the course of work were selected and optimized protocols for the synthesis of clusters of two spectral types. The lifetimes of the order of one or two nanoseconds correlate with published data, however, were found and more long-lived states, which are of particular interest for further study.

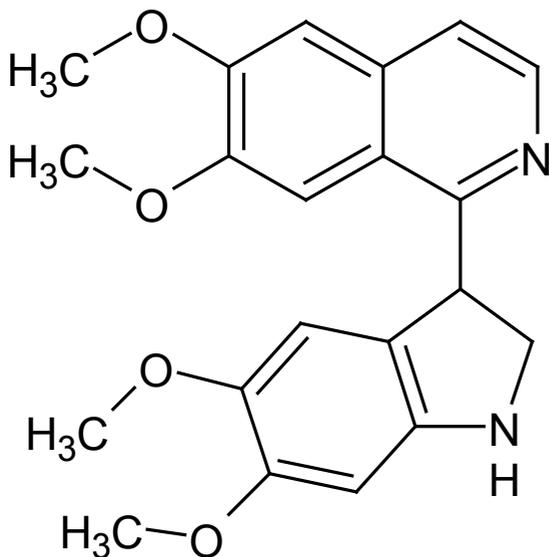
Thermodynamics of the interaction of DNA molecule with papaverine analogue containing indole substitute

Travkina Veronika, Osinnikova Daria
travkinaveronika@gmail.com

Scientific supervisor: Dr. Moroshkina E.B., Department of Molecular Biophysics, Faculty of Physics, Saint-Petersburg State University

Knowledge of the thermodynamic parameters of the equilibrium DNA complexes with various low molecular weight biological active compounds is necessary for development of new drugs whose mechanism of action is associated with the formation of equilibrium complexes. The main methods of determining the thermodynamic binding parameters, such as the binding constant and the number of binding sites, are spectrophotometry and microcalorimetry. However, standard methods of titration used in both cases are different, which may affect the results.

In this work the interaction of DNA with the isoquinoline derivatives having indole substitute in the first position (Fig. 1), which is similar to the well-known drug papaverine, was studied by the methods of spectrophotometry, microcalorimetry and circular dichroism.



Spectral and calorimetric studies were carried out in parallel and showed that this compound binds to the DNA in two ways: as a monomer and as a dimer. The spectral characteristics of the monomer linked compound were identified, as well as the enthalpy of its interaction with DNA and interaction between the monomers located at the nearest binding sites. The obtained results

Fig. 1. Isoquinoline derivatives with indole substitute in the first position.

are consistent with the intercalation binding model.

This work was partially carried out in the RC SPSU "Thermogravimetric and Calorimetric Research Center".

I. Resonance Phenomena in Condensed Matter

Self assembly processes of biodegradable surfactants as studied by NMR

Dmitriev Roman
dmitriev.rs@gmail.com

Scientific supervisor: Prof. Dr. Chizhik V.I., Department of Nuclear-Physical Methods of Investigation, Faculty of Physics, Saint-Petersburg State University

Surfactants currently have a wide range of applications in various industries and households. For example, surfactants are used as agents in the flotation process in wastewater treatment at refineries. As the result, the surfactants are contained in industrial, as well as domestic, water refineries. In this aspect, one of the major goals of the modern science is to create biodegradable surfactants while retaining their highly effective physico-chemical properties. In the practical application of surfactants the mixtures of amphiphilic substances are commonly used. Some of the most important properties of sarcosinates: they are very well compatible with other surfactants and are characterized by rapid biodegradation.

To study the processes of self-assembly of amphiphilic molecules, the NMR method can be considered as the most informative one [1]. The main feature of the NMR-method is the possibility to obtain data on the system without the addition of recording labels. Measuring the independent parameters of a system (such as NMR-relaxation times, self-diffusion coefficients of individual components) and spectral characteristics one can draw conclusions about the static and dynamic characteristics of the system, as well as the kinetics of exchange processes: conformational transitions, exchange of atoms.

In this work we have investigated the water-deuterated solutions of sodium laurylsarcosinate (SLS, $C_{15}H_{28}NO_3Na$) in the ranges of concentrations $c = 0,007 \div 0,19$ mol /l and temperatures from 293 to 343 K. All the measurements were carried out on spectrometers company "Bruker" in the "Magnetic Resonance Research Centre" of St. Petersburg State University. The temperature dependence of the internal chemical shifts of 1H and ^{13}C showed that in the region of 55-60°C there was the restructuring of micellar aggregates. It is evident from the relaxation data that trans-isomers are more mobile in the monomeric state, as well as the micellar groups NCH_2 and NCH_3 . The hydrodynamic radii of the micelles obtained from diffusion data were in two times bigger than the length of the SLS molecule. This confirms the assumption that the micellar form differs from spherical, even at concentrations close to the CMC. The increase in the temperature does not change the ratio of trans- and cis-isomers in solution, that is, the collapse of the micelles of SLS does not occur in the temperature range studied.

References

1. O. Soderman and P. Stilbs. // Progress In Nuclear Magnetic Resonance Spectroscopy, 26(5), 445–482, 1994.

Concentration effect on ^7Li quadrupolar relaxation in LiCl aqueous solutions: a molecular dynamics simulation study

Egorova Mariia
maryaverina@gmail.com

Scientific supervisor: Prof. Dr. Chizhik V.I., Department of Nuclear-Physics Research Methods, Faculty of Physics, Saint-Petersburg State University

Understanding the microstructure of liquid systems is a problem of fundamental interest in physical chemistry. To describe the peculiarities of various physico-chemical processes at the molecular level is extremely important to explain macroscopic properties of liquids. It would be also very fruitful for the development of solution chemistry and related fields (electrochemistry, biochemistry, etc.). One of the most puzzling group of liquid substances is concentrated multi-component aqueous electrolyte solutions. The dominant characteristic of any concentrated solution is a high concentration of solvents and a relatively low content of water.

Nuclear magnetic relaxation is an important source of information on structural and dynamic properties of liquid systems. However, in such experiments we can measure macroscopic characteristics only. To get directly any reliable information on the microscopic properties of solutions is a complicated task. The variety of simultaneous molecular processes in solutions (microheterogeneity, complexation, dissociation, etc.) do not allow anyone to connect unambiguously experimental relaxation data with microscopic characteristics. As a result, different interpretations of the same relaxation data can be in poor agreement with each other.

As a main tool for studying relaxation processes in concentrated multi-component aqueous electrolyte solutions we have chosen molecular dynamics computer simulations. Simulations allow us to obtain detailed information on structure and kinetic of any solution at the molecular level. However, we should take into account that all interatomic interactions are described by model potentials. Therefore, it is always necessary to calculate macroscopic characteristics of a solution in order to compare with the experimental ones and test the quality of models used.

To investigate the nature of quadrupolar relaxation in multi-component systems in detail, the classical molecular dynamics simulations of LiCl aqueous solutions were carried out over the wide concentration range (1.0-18.5 mol/kg) at normal conditions. Times of rotational reorientation of water molecules in different solutions substructures, values of z-component of the electric field gradient at the location of lithium cation and corresponding ^7Li quadrupolar relaxation rates were calculated and compared with the available experimental data.

The financial support of the Russian Foundation for Basic Research (grant 13-03-01073), and Saint-Petersburg State University (grant 11.0.63.2010) are gratefully acknowledged.

Principles of dynamic nuclear polarization in a low magnetic field

Furman Dmitry
dm.furmannmr@mail.ru

Scientific supervisor: Dr. Frolov V.V., Department of Nuclear-Physics Research Methods, Faculty of Physics, Saint-Petersburg State University

Contrast enhancement of images is an important task for MRI scan. You can increase the signal-noise ratio using the method of dynamic nuclear polarization (additional irradiation of the sample with the frequency of ESR). However, the frequency of the polarizing pulse for most MRI scanners (more than 1 T) is equal to a few hundred gigahertz, which destroys many organic substances and dangerous for living organisms.

The use of weak fields on the order tens of mT allows you to use the polarizing pulse order of hundreds of MHz, which is more secure. Experiments DNP in MRI are able to pass under normal temperature conditions without strong cooling investigated object of study. Method contrast is that the places where the application of this radical DNP MR image is more intense signal (from the hydrogen nuclei). DNP method is applicable to the nuclei ^{13}C , ^{15}N , ^{31}P and ^1H . Observed improved signal / noise ratio, as well as the ability to use both the spin echo (SE) and gradient echo (GRE) for space encoding.

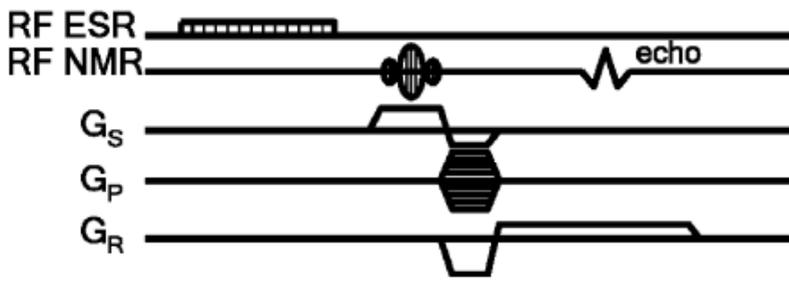


Fig. 1. DNP MRI protocol (from [1]).

References

1. A. Milton Franklin Benial 1, Kazuhiro Ichikawa, Ramachandran Murugesan, Ken-ichi Yamada, Hideo Utsumi // Journal of Magnetic Resonance 182 (2006) 273–282.
2. Mark D. Lingwood, Ivan A. Ivanov, Alissa R. Cote // Journal of Magnetic Resonance 204 (2010) 56–63.

Diffusion NMR imaging in magnetic field 7 mT

Ievleva Svetlana, Luzhetckaia Nadezhda
ievlevasvetlanka@mail.ru

Scientific supervisor: Dr. Frolov V.V., Department of Nuclear-Physical Research Methods, Faculty of Physics, Saint-Petersburg State University

The possibility of using MRI diagnostic imaging technique of internal human organs based on the high water content in the human organism. Diffusion weighted imaging (DWI) is one of new effective versions of MRI. As a rule, such researches are performed on medical MR scanners in high magnetic field (1-3 T and more) [1]. In this report the results of experiment on obtaining DWI in very low magnetic field (7 mT) are presented, using the laboratory homebuilt nuclear magnetic resonance imager in department of Nuclear-Physical Research Methods. The equipment of magnetic resonance imaging of DWI allows us to construct a map of molecular diffusion rates (as a rule, water molecules) in biological tissues as *in vivo* and *in vitro*. The features of water molecules diffusion can be explained with features of tissues structure. For medicine the great interest is presented in those cases when DWI of a normal tissue differs from the pathologically changed.

The method of obtaining DWI represents a combination of methods to measure self-diffusion coefficient and methods of spatial encoding in MRI [2, 3]. For realization of the imaging pulse sequence the special program was created in the LabView environment.

References

1. V. Perrin. MRI Techniques. Wiley, 2013. -225 p.
2. N. Luzhetckaia, S. Ievleva. NMR measurement of selfdiffusion in low magnetic field// Abstracts the 5th International Student's Conference "Science and Progress", November, 10-14 (2014) Saint-Petersburg, Petergof, Russia.
3. M.A. Bernstein, K.F. King, X.J. Zhou. Handbook of MRI Pulse Sequences. Elsevier, Oxford, 1015 p. (2004).

A magnetic field mapping for MRI scanner at 7 mT

Ivanov Viacheslav
ivi-lamer@rambler.ru

Scientific supervisor: Dr. Frolov V.V., Department of Nuclear Physics Research Methods, Faculty of Physics, Saint-Petersburg State University

Problem of static magnetic field homogeneity and getting spatial distribution of the field has always been an urgent problem in NMR spectroscopy and imaging. Conventional method of field scanning realized by small-size sample moving through the volume of magnetic system and point-by-point field measuring is time-consuming, not accurate and requires special equipment, therefore such methods which present field map of the whole sample or at least its section after computer processing of NMR data are an object of interest. Such methods can be developed on the basis of NMR imaging techniques.

In this work one of these methods was realized. As a result magnetic field map at low-field (7 mT) MRI scanner on cylindrical sample was obtained.

The hydration layer around the B1 domain of immunoglobulin-binding protein L and water proton magnetic relaxation. A molecular dynamics simulation study

Krylova Ekaterina
krylovaea2803@mail.ru

Scientific supervisor: Dr. Egorov A.V., Faculty of Physics, Saint-Petersburg State University

Understanding the properties of water in biological systems is a problem of fundamental interest in chemistry and biology. The water-protein interaction is a major determinant of protein folding and conformational stability. In the present study the structure of the hydration layer that surrounds the B1 domain of immunoglobulin-binding protein L (PDB code 2PTL [1]) as well as the dynamics of water molecules in the layer has been examined using molecular dynamics computer simulations.

A model solution of 1 protein molecule (963 atoms) among 7404 water molecules was considered. Simulations were carried out in an isothermal-isobaric ensemble in a cubic periodic cell at 1 atm and 25°C using the *MDynaMix* package [2]. To describe water molecules the SPC/E model [3] was employed. To describe water interactions with the protein molecule the force field by Cornell et al. [4] was used. The temperature was kept constant by using Nose-Hoover thermostat and pressure was regulated by Hoover barostat. The equations of motion were solved using the Verlet algorithm with a time step of 2.0 fs. The Coulomb interactions were calculated using the Ewald summation method. The SHAKE procedure was employed to constrain all the bond lengths. The system was equilibrated during a 30 ps run. Further, a 100 ps simulation was performed.

A detailed microscopic picture of protein surface hydration structure was obtained by calculating radial distribution functions (RDFs) between protein α -carbons and water oxygens. On the basis of the analysis of RDFs the thickness of the hydration layer was estimated. To describe dynamics of protein hydration the residence times of water molecules in various regions of the hydration layer was calculated following the standard procedure described in [5].

This work was supported by the grant of the Russian Foundation for Basic Research (13-03-01073-a). The authors also acknowledge Saint-Petersburg State University for a research grant 11.0.63.2010.

References

1. J.W. O'Neill, D.E. Kim et al. // *Acta Cryst. D*, 57, 480-487 (2001).
2. A.P. Lyubartsev, A. Laaksonen // *Comp. Phys. Comm.*, 128, 565-589 (2000).
3. H.J.C. Berendsen, J.R. Grigera, T.P. Straatsma // *J. Phys. Chem.*, 91, 6269-6271 (1987).
4. W.D. Cornell, P. Cieplak, C.I. Bayly, et al. // *J. Am. Chem. Soc.*, 117, 5179-5197 (1995).
5. R.W. Impey et al. // *J. Phys. Chem.*, 87, 5071-5083 (1983).

NMR measurement of selfdiffusion in low magnetic field

Luzhetckaia Nadezhda, Ievleva Svetlana
jennet24@mail.ru

Scientific supervisor: Dr. Frolov V.V., Department of Nuclear-Physical Research Methods, Faculty of Physics, Saint-Petersburg State University

Magnetic resonance image (MRI) at very low field more and more becomes widespread subject of research (for example [1, 2]). One of important informative MRI-techniques is a visualization of spatial distribution of self-diffusion coefficient (diffusion-weighted imaging, DWI). However, to create DWI it requires a special technique to determine the diffusion coefficient. The technique is usable in high-field nuclear magnetic resonance (NMR) but its implementation at very low magnetic field presents some difficulties.

Here we present elaboration and realization of the method of diffusion coefficient measurement using the low-field (7 mT) homebuilt NMR imager. NMR is unique technique that enables to study chaotic movement of molecules through measurement of the self-diffusion coefficient. It should be noted that such measurements are performed without using any radioactive labels (which are employed in traditional methods of physical chemistry). Required conditions for measurement of self-diffusion coefficient are a presence of a sample containing molecules with nuclei, which possess a non-zero spin and magnetic field in which the sample is put. Self-diffusion coefficients in model systems were measured with Hahn Echo pulse sequence in the presence of a magnetic field gradient [3, 4].

Thereby, the possibility of using weak magnetic fields of the order of several milliteslas for practical diffusion measurements using NMR techniques was shown.

References

1. V.S. Zotev, T. Ownes et al. //JMR, v.207 №1, pp. 78-88 (2010).
2. M.E. Halse, A. Coy et al. //J. Magn. Res. v. 182, pp. 75-83 (2006).
3. А.А. Вашман, И.С. Пронин – Ядерная магнитная релаксационная спектроскопия. -М.: Энергоатомиздат, 232 с. (1986).
4. В.И. Чижик - Ядерная магнитная релаксация, СПб: Изд-во С.-Петерб. ун-та, 388 с. (2004).

Magnetic resonance study of atomic hydrogen and deuterium stabilized in solid H₂ and D₂ matrices below 1K

Sheludiakov Sergey
seshel@utu.fi

Scientific supervisor: Dr. Vasiliev S., Department of Physics and Astronomy, University of Turku, Finland

Hydrogen and deuterium solids at low temperatures represent a special class of quantum crystals, where due to the large zero point oscillations and light mass, the effects of quantum tunnelling play an important role. Behaviour of atomic impurities in these crystals attracts special attention due to a possibility of reaching collective quantum phenomena related with Bose-Einstein Condensation (BEC) or so-called supersolid behaviour. This may happen at high enough densities of atomic hydrogen. In our previous work we succeeded in reaching record high densities of atoms: $4 \cdot 10^{19} \text{cm}^{-3}$ [1]. This was done by implementing a novel method of in-situ dissociation of hydrogen molecules by low temperature (<1 K) RF discharge. H and D are the simplest atomic systems where magnetic resonance methods may be utilized for the characterization of the sample properties. In this work we present the first ESR study of H/D-impurities stabilized in solid H₂ and D₂ matrices below 1K.

We found out that quantum isotopic exchange reactions $\text{D} + \text{H}_2 = \text{H} + \text{HD}$ and $\text{D} + \text{HD} = \text{H} + \text{D}_2$ go with high enough rate at temperatures below 1K and effectively increase the concentration of atomic hydrogen in H;D; H₂;D₂ mixture films. Efficient dynamic nuclear polarization (DNP) of H in D₂ matrices was created via both Overhauser and solid effects. We suggest that interaction of electrons of the H atoms with magnetic moments of ortho-D₂ molecules greatly enhances the probabilities of forbidden transitions. The presence of D₂ molecules in a close neighbourhood of H and D atoms was supported by observation of the holes in both ESR spectra of H and D atoms during pumping the position of the satellite lines which appear due to simultaneous spin flips of the electron of the atom and the deuteron spin on a neighbouring D₂ molecule. In addition, pumping the center of the H spectrum created negative DNP. All attempts to observe DNP via the solid effect and pumping the center of the spectrum in pure H₂ were unsuccessful. We discuss possible explanations of this effect being due to the nuclear polarization transfer between H and D, or strong exchange effects between clusters of H atoms.

References

1. J. Ahokas, O. Vainio, S. Novotny, V.V. Khmelenko, D.M. Lee and S. Vasiliev //Phys. Rev. B, vol.81, 104516, (2010).

Hydrogen self-diffusion processes in the lattice of transitional metal alloys

Vyvodtceva Anna, Bavrina Olga
annavyvod@gmail.com

Scientific supervisor: Dr. Shelyapina M.G., Department of Nuclear-Physics Research Methods, Faculty of Physics, Saint-Petersburg State University

Metal hydrogen systems have been extensively studied last decades due to their ability to be used as hydrogen storage materials. A good hydrogen storage material has to fulfill a number of criteria, such as a high hydrogen storage capacity, a low hydrogen desorption temperature, a high hydrogen sorption kinetics, a reversibility of the hydrogen sorption reaction etc. These properties, in their turn, are determined by metal-hydrogen bonding and potential energy pattern that govern both the static (distribution of hydrogen atoms over the interstitial sites) and dynamic (hydrogen self-diffusion) properties.

Nuclear magnetic resonance (NMR) has approved itself quite valuable for studies both the hydrogen location and mobility in metals. The activation energy of hydrogen self-diffusion process (E_a) can be determined either from proton spin-lattice relaxation experiments or from diffusivity measurements.

On the other hand, E_a can be calculated implicitly using the density functional theory (DFT) method. In the initial alloys of studied hydrides the distribution of the Ti, V and Cr atoms over both sites of the bcc lattice is random. Disordered systems can be studied by Korringa-Kohn-Rostoker method with coherent potential approximation (KKR-CPA).

In this work we report on the results of hydrogen self-diffusion coefficient measurements in ternary Ti-V-Cr alloys of various compositions using NMR method. The said KKR-CPA stability research is also represented. The hydrogen diffusion measurements have been performed employing the static field gradient nuclear magnetic resonance method (SFG NMR) [2].

All hydrides exhibit rather slow hydrogen diffusion ($D = 1\div 3 \times 10^{-11} \text{m}^2/\text{s}$). 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 are in fair agreement with the results obtained from our earlier relaxation studies [4]: 0.15 and 0.12 eV for $\text{TiV}_{0.8}\text{Cr}_{1.2}$ and $\text{Ti}_{0.5}\text{V}_{1.9}\text{Cr}_{0.6}$, respectively.

References

1. S. Miraglia et al. // J. Alloys Compd. 442, 49 54 (2007).
2. I. Chang, F. Fujara, B. Geil // J. of Non-Crystalline Solids, 172-174, p. 674-681 (1994).
3. M. Shelyapina et al. // Phys Solid State 49(3), 399 402 (2007).

Nuclear polarization and relaxation in Si:P at ultra-low temperatures

Zvezdov Denis
denis.zvezdov131@gmail.com

Scientific supervisors: Prof. Dr. Vasiliev S., Department of Physics and Astronomy, Faculty of Natural Sciences, University of Turku, Finland, Prof. Dr. Tayurskii D., Institute of Physics, Kazan Federal University, Kazan, Russia.

Dynamic nuclear polarization (DNP) is an important tool in magnetic resonance, which provides versatile control of the nuclear polarization and substantial enhancement of the sensitivity of NMR. Very interesting systems where the effects of DNP can be studied are shallow donors (P, As, Bi) in Si. Magnetic resonance studies of these samples have a long history starting from pioneering work of Feher [1]. Recently the interest to this system has been raised by the proposal of Kane [2] to utilize these impurity atoms for quantum computing with the nuclear spin serving as a memory qubit and electron spin for readout.

In this work we report on the details of the experimental study of DNP of ^{31}P donors in silicon (Si:P) performed in strong magnetic field and temperatures below 1K. At these conditions donor electron spins are fully polarized, electron and nuclear relaxation times are extremely long. All these factors substantially change the efficiency of DNP: pumping with extremely low RF powers ($<1\ \mu\text{W}$) for reasonably short time (≈ 1 hour) very high values of DNP ($>98\%$) of ^{31}P were reached. The DNP has been obtained via the Overhauser effect by pumping allowed ESR transitions followed by the cross relaxation via the flip-flip and flip-flop transitions. We evaluated the corresponding cross relaxation times and discuss the dependence of the DNP on the pumping time.

We performed detailed study of the nuclear relaxation of ^{31}P donors in the temperature range 0.75-2 K. The relaxation did not follow a single exponential dependence of time, but is quite well described by the bi-exponential function. Both relaxation times have exponential dependence on $1/T$ with the electron Zeeman energy in the exponent, which indicates on the Nuclear Orbach mechanism of relaxation.

We also realized a resolved solid effect in Si:P by pumping the ^{31}P - ^{29}Si forbidden electron-nuclear transitions. As a result we observed a pattern of narrow holes and peaks in the ESR spectrum, corresponding to polarization of ^{29}Si in the specific lattice sites, resolved due to the superhyperfine interactions ^{31}P - ^{29}Si . This opens a way of using large ensembles of identical ^{29}Si nuclei for quantum computing.

References

1. G. Feher // Phys. Rev. 114, p. 1219 (1959).
2. B.E. Kane // Nature 393, p.133 (1998).

S. First Steps in Science

DNA complexes with coordination compounds containing phthalocyanines and their stability in water solution

Dyachkova Olga
eliondo@mail.com

Scientific supervisor: Prof. Dr. Kasyanenko N.A., Department of Molecular Biophysics, Faculty of Physics, Saint-Petersburg State University

The metallized diphtalocyanines (PC) are well known biologically active compounds with a wide range of applications from medicine to microelectronics. Diphtalocyanines can be used as catalysts for redox reactions.

Good solubility of drugs in a water is a necessary condition for medical use. Usually they are first dissolved in dimethylsulfoxide. Then the gradual addition of water into solution transforms the system to the form suitable for the application during medical procedures.

The problem of the stability of these solutions requires the right decision. This is especially important when studying the interaction of these compounds with DNA molecule in solution. This work was devoted to the consideration of the problem.

The aim of the study is to examine the properties of PC solutions in time. The analyze DNA-PC interaction was also done.

It was shown that the addition of DNA into PC solutions causes the formation of DNA-PC complexes. DNA molecule stabilizes the solution of PC.

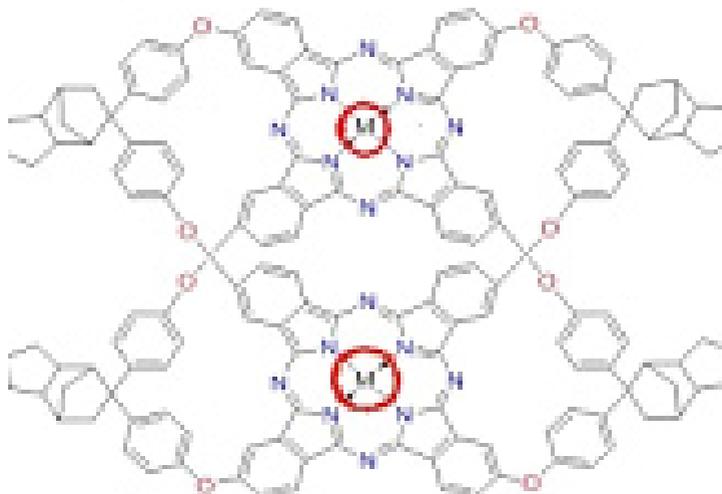


Fig. 1. Structure of diphtalocyanines (PC).

Optical spectra of excitons in high-quality quantum well

Makarova Oksana
oksansha@gmail.com

Scientific supervisor: Grigoryev P., Department of Solid State Physics, Faculty of Physics, Saint Petersburg State University

Any object of a nanometer size made of semiconductor material is called semiconductor nanostructure. The quantum well (QW) is the simplest example of a nanostructure. One can make a QW placing a layer of one semiconductor crystal in between of two crystal layers of different compound.

QW allows one to realize the simple square potential model of quantum mechanics. Each layer of a semiconductor has a band gap in its energy diagram, and allows two types of carriers: electrons in the conduction band and holes in the valence band. Band offset of the middle semiconductor layer differs from that of two surrounding layers, called barriers. The energy diagram of conventional QW usually forms a square potential well for both electron and a hole.

The states of electrons and holes are described by Schrödinger equation. Its solution for the square potential are standing waves [1]. However, both electron and hole have charges, therefore they are attracted to each other by the Coulomb force. This attraction changes wave functions and energies of the carriers; the system becomes similar to hydrogen atom.

We studied reflectance and photoluminescence spectra of the sample with 250 nm QW made of GaAs surrounded by AlGaAs barriers. In the experiments the sample was put in the cryostat at 4K temperature. We measured for the sample excited by a laser or white light source using a monochromator. In our case, each peculiarity corresponds to the energy of carriers in QW. Electrons and holes, created by the laser light, relax down to states in a QW, then decay and emit light.

In our report we analyze the energies of peculiarities and attribute them to the theoretically predicted states. Additionally, we analyze the width of photoluminescence peaks. In high-quality structures the peaks are not broadened by the QW width fluctuations, the width corresponds to the lifetime of the radiating state. We plan to investigate the magnetic properties of an exciton in a QW, and the peaks widths are critical in studying the magnetic field splittings.

References

1. J.H. Davies. The Physics of Low-Dimensional Semiconductors. Cambridge: Cambridge University Press, 1998.

The study of three-component complex (DNA, surfactant, phthalocyanine) stability *in vitro*

Riazantseva Valentina
rvmari39@mail.ru

Scientific supervisor: Prof. Dr. Kasyanenko N.A., Department of Molecular Biophysics, Faculty of Physics, Saint-Petersburg State University

Gene vector - is a molecular complex that is formed to facilitate penetration of recombinant DNA through the cell membrane. The recombinant DNA is the construction which must be designed for the transfection of new gene into target cell. The first step for the construction of gene vector is the preparation of system for the compaction of DNA coil in the solution. Gene vectors can be used also for the targeted delivery of the drugs.

Metal complexes of phthalocyanines can be used as active agents during the different medical applications. One of the difficulties of manipulation with such systems in practice is the probable lack of stability. Indeed, the phthalocyanines in a water solutions have usually a tendency to precipitate. This greatly complicates their use in practice. The formation of DNA complexes with phthalocyanines prevents the precipitation of drugs from the solution. For the formation of complex gene vector DNA- phthalocyanines it is necessary to find the optimal way for DNA packaging in a solution.

We use cationic surfactant with UV-sensitive azobenzene group (Fig. 1) for the packaging of DNA molecule. The compound was obtained in the laboratory of Professor S. Santer (Potsdam University, Germany).

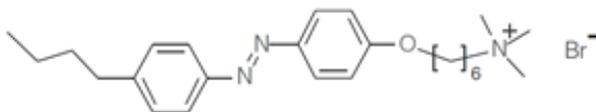


Fig.1. Surfactant molecule.

The first step of our research was the investigation of DNA-surfactant interaction. Surfactant solution was mixed with the solution of high molecular DNA ("Sigma" (M = 8.8 MDa). The irradiation of surfactant solutions with UV light (365 nm) causes trans-cis conformational transition of compound. The visible light (400 nm) can induce cis-trans transition. It is known that the addition of surfactant into DNA solution causes DNA condensation. UV and visible light can transform DNA –surfactant complex.

We use different metal complexes of phthalocyanines (PC), such as SuPC, NiPC, CoPC. The stability of DNA complexes with PC and surfactants was studied. It was found that metal complexes of PC bind to DNA in the presence of surfactants. Complexation does not prevent multiple trans-cis-trans isomerization of the surfactant. This result confirms the stability of this three-component system.

IR study of ozone adsorbed on CaF₂

Sivokhina Maria, Belykh Roman
mjafamjau@gmail.com

Scientific supervisor: Prof. Dr. Tsyganenko A.A., Department of General Physics 2, Faculty of Physics, Saint-Petersburg State University

Ozone plays an important role, forming protective layer in upper atmosphere. But in troposphere it is mostly regarded as a rather toxic active radical, affecting human health. In marine regions, sea aerosols, consisting of microcrystals of ice and various salts, were reported to adsorb ozone and conduct photocatalytic reactions, as well as heterogeneous reactions, producing bromine radicals, highly active in ozone destruction [1].

In the present paper we report a study of molecular ozone adsorption and transformation on the pellets of microcrystalline CaF₂ under UV light by means of FT-IR spectroscopy. Fig. 1 shows the spectrum of a pellet after adsorption of increasing amounts of O₃ at 77 K and subsequent irradiation by UV light. The

bands at 1113 and 1034 cm⁻¹ due to the stretching vibrations of ozone molecules are similar to those previously observed after ozone adsorption on oxides [2]. UV irradiation leads to decrease of these bands and growth of a new one at 1060 cm⁻¹, providing evidence for the degradation of adsorbed molecules with the formation of some new surface species. To establish the structure of the latter and to clarify the mechanism of the observed photo-stimulated reaction further experiments are planned, including the use of ¹⁸O isotopically labeled ozone and

investigation ozone adsorption on different salts typical of natural sea aerosols.

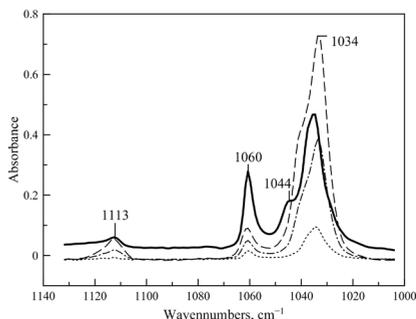


Fig. 1 FTIR spectra of ozone adsorbed on disperse CaF₂ at 77 K. Dashed lines – upon increasing coverage, solid line – after 15 min UV irradiation.

References

1. B.J. Finlayson-Pitts, F.E. Livingston, and H.N. Berko // Nature, 343, 622-625, 1990.
2. A.V. Alekseev, M.A. Babaeva, D.S. Bystrov, A.A. Tsyganenko and V.A. Yushkov. All-Union Symp. On Photochemical Processes in the Earth Atmosphere, Moscow, 1986, Tchernogolovka, 1986, p. 27.
3. K.M. Bulanin, J.C. Lavalley, A.A. Tsyganenko // Colloids and Surfaces, 101, 153-158, 1995.

Ionocraft – high voltage capacitor

Sviridov Alexander
alex777sv@gmail.com

Scientific supervisors: Dr. Gordeev E.I., Department of Earth's Physics, Faculty of Physics, Saint-Petersburg State University and Dr. Chirkov V.A., Electrophysics Research and Education Center, Faculty of Physics, Saint-Petersburg State University

Combination of the well-known physical phenomena, such as corona discharge and ionic wind, leads to exciting effect – high voltage levitation of asymmetrical capacitors (called Lifters). In spite of the clear physics behind, there is still a lot of speculation and contradiction in literature about the basic characteristics of lifters and even the levitation origin. To take a closer look at this phenomenon we construct the experimental model of the ionocraft and try to determine its main physical characteristics. First of all we empirically derive dependence of lifting force on the electric current and voltage observed in our system. Obtained results were compared with theoretical estimations and other empirical results available in literature.

DNA absorption spectra in complexes with anticancer drugs cisplatin, carboplatin, and a novel compound BP- C1

Vergasova Ekatherina
katevergasova98@gmail.com

Scientific supervisor: Prof. Dr. Kasyanenko N.A., Department of Molecular Biophysics, Faculty of Physics, Saint-Petersburg State University

One of the main problems of modern medicine is the search for new anticancer drugs with high efficacy and low toxicity. It is known that the effect of anticancer drugs based on platinum is realized due to their binding to DNA in the cell and inhibition of replication. Study of DNA interaction of with antitumour drugs in a solution (in vitro) is a widely used test for their biological activity. Indeed, the aqueous medium is a natural environment for DNA-drug binding *in vivo* (in living systems).

The aim of this work is to answer the question whether the new drug interacts with the DNA in a solution. Furthermore, a comparison of new compound BP-C1 and well known anticancer drugs was done. We use anticancer compounds: cis-dihlorodiamminplatinum (II) (the pharmacological name is cisplatin), and 1,1-cyclobutane dicarboxylato diammineplatinum (II) (carboplatin) (see Fig. 1A and B). BP-C1 is completely new compound. The exact structure BP-C1 is unknown. All three drugs are the coordination compounds of platinum.

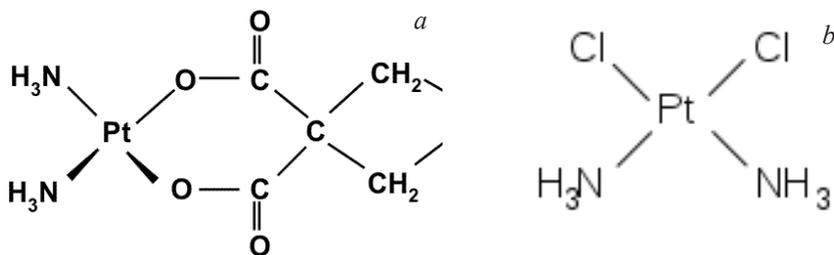


Fig.1. Carboplatin (A) and cisplatin(B).

It was shown that DNA interaction with cisplatin and carboplatin causes changes in DNA absorption spectrum, which indicates the effect of binding on secondary structure in macromolecule. Cisplatin causes a small shift of the maximum of absorption band to the long wavelength region, hyperchromic effect and changing the shape of the band. Carboplatin induces only the appearance of hyperchromic effect during the binding to DNA. BP-C1 also interacts with DNA. The binding is accompanied with transformation of DNA absorption spectrum. The analysis of spectral data shows that the binding of BP-C1 with DNA differs from DNA-cisplatin interaction.

Table of Content

Organizing Committee

Heads of sections

Invited Lections 5

XMCD: a Versatile, Element Specific Method for Studying Magnetism in Multi-Component Systems

Kai Fauth 6

Electron spin polarimetry for spin resolved photoemission

O.E. Tereshchenko 7

Synchrotron Radiation: Production, Properties, and Uses

Hartmut Zabel 8

German-Russian Interdisciplinary Science Center (G-RISC)

Prof. Dr. Eckart Rühl, Natalia Kolanovska 9

Russian-German Laboratory at BESSY II, Berlin

Dmitry Marchenko Eckart Rühl 10

Nonlocal Problems for Vlasov-Poisson Equations with External Magnetic Field in Infinite Cylinder

Alexander Skubachevskii 11

Reaction-diffusion systems with hysteresis

Pavel Gurevich 12

A. Chemistry 13

Solid-state luminescence of Au(I), Ag(I) and Cu(I) complexes with tetradentate phosphine ligand

Beliaev Andrei 14

Synthesis of B-homo analogues of steroid estrogens

Drozдов Andrey 15

Prospects of biodiesel production using coupled processes

Golikova Alexandra, Toikka Maria 16

Rhenium (I) diimine complexes with extended chromophoric phosphines <i>Kisel Kristina</i>	17
The activation mechanism of gold for oxidation reactions <i>Klyushin Alexander</i>	18
Synthesis of 5-amino-1,2,4-oxadizoles via Zn ^{II} -catalyzed reaction of amidoximes and cyanamides <i>Kulish Kirill</i>	19
Quantum-chemical simulation of the interaction of phenols with potassium carbonate in the presence of hematite <i>Lyutkin Andrew</i>	20
Photochemistry of Copper(II) Chloro complexes in Acetonitrile Studied by Means of Femtosecond Transient Absorption Spectroscopy <i>Mereshchenko Andrey, Pavel Olshin</i>	21
Structural and optical properties of glasses A ₂ O-P ₂ O ₅ -Nb ₂ O ₅ (A=Li, Na, K) <i>Olshin Pavel, Vasil'eva Anna, Kireev Alexey, Manshina Alina, Sokolov Ivan</i> .	22
A new method for the isolation and concentration of the herbicide glyphosate and its major metabolite aminomethylphosphonic acid <i>Shreyner Ekaterina</i>	23
Influence of industrial pollutions on a chemical composition and morphology of some medicinal plants <i>Solovyeva Natalia, D.M. Toropova, Y.G. Oleneva, A.I. Ivanova, S.D. Khizhnyak, P.M. Pakhomov</i>	24
B. Geo- and Astrophysics	25
Interference seismic waves <i>Bazulin Maksim</i>	26
Analysis of the observations of CO ₂ concentrations in the ambient air at the Peterhof station <i>Foka Stefani</i>	27
Gydra - GPU-based code for astrophysical SPH simulations <i>Korsunov Igor</i>	28
Spectral properties of the X-ray binary GX339-4 <i>Kosenkov Iliia, Zabelina Natalia</i>	29

Spectral characteristics of sources located above the neutral line of the photospheric magnetic field and their connection with flares <i>Kurochkin Evgenii</i>	30
Russian aeromagnetic exploration and complex airborne geophysics at the start of a new phase – use of unmanned aviation vehicles <i>Kuznetsova Anna</i>	31
Photometry and polarimetry of supernovae performed on telescopes LX200 and AZT-8 <i>Mokrushina Anna</i>	32
Correlation of radial fluctuations in deep galaxy redshift surveys <i>Shirokov Stanislav</i>	33
The Spatial Distribution of Galaxies in 2MRS and SDSS Catalogs <i>Tekhanovich Daniil</i>	34
Estimation of Lamé parameters for the two-dimensional elasticity equations <i>Valitov Aleksandr</i>	35
C. Mathematics and Mechanics	37
Local bifurcation for discrete-time non-autonomous systems connected with a heart model <i>Abdalova Iuliia</i>	38
Topology preserving algorithm for cartographic generalization <i>Alexeev Vladislav, V. Bogaevskaya, A. Gorokhov, V. Knyazev, M. Preobrazhenskaia, A. Ukhalov, H. Edelsbrunner, O. Yakimova</i>	39
Controlling the controller: hysteresis-delay differential equations <i>Eyal Ron</i>	40
Andronov–Hopf bifurcation in equation with inconstant delay <i>Golubenets Vyacheslav</i>	41
Andronov-Hopf bifurcation of one or more cycles in the Mackey-Glass type delay differential equation <i>Ignatenko Vera</i>	42
Homogenization of the first initial-boundary value problem for parabolic systems: L_2 -operator error estimates <i>Meshkova Yulia</i>	43

Numerical probabilistic approach to solution of the Cauchy problem for quasilinear parabolic equations <i>Nemchenko Ekaterina</i>	44
Shadowing for systems without transversality <i>Petrov Aleksey</i>	45
Control of synchronization in neural delay-coupled networks with heterogeneous threshold parameters <i>Plotnikov Sergei</i>	46
Monte Carlo Simulation for Stochastic Differential Equations <i>Pogosian Anna</i>	47
Application of the Method of Quasi-Normal Forms to the Mathematical Model of a Single Neuron <i>Preobrazhenskaia Margarita</i>	48
Simulations of high-velocity star motions in the Galactic gravitational field <i>Shirokova Kseniia</i>	49
Preprocessing of endoscopy images <i>Symanovich Maksim</i>	50
Caratheodory dimension of invariant sets for dynamical systems with multiple time <i>Voynov Dmitriy</i>	51
E. Applied Physics	53
Gas-separating membranes based on polyimides of variable structure <i>Antipov Mikhail</i>	54
Effect of the solution parameters on the characteristics of the Ag nanoparticles obtained by method of direct laser synthesis <i>Leonova Iuliia</i>	55
Light control over plasmon properties of gold nano-particles <i>Lysyakova Liudmila</i>	56
Research of consequences of the accidents at nuclear power plants and impact on the environment of Leningrad region <i>Merzlaya Anastasia</i>	57

Manipulation azobenzene containing surfactant via far – and nearfield <i>Johann Nuck,¹ Burhard Stiller,¹ Yuri Petrov², Vladimir Mikhailovskii², Oleg Vyvenko,² Svetlana Santer¹</i>	58
Study of the characteristics of neutron scintillators <i>Safulina Irina</i>	59
Manufacturing and testing an electrochemical cell for the anodic oxidation of titanium <i>Starodubtseva Lyudmila.....</i>	60
Velocity spread in quantum hydrodynamics <i>Zippa Andrey.....</i>	61
D. Solid State Physics.....	63
Nuclear spin relaxation in bulk and nanostructured sodium <i>Antonenko Anastasiia.....</i>	64
Simulation of quantum yields of heterogeneous processes <i>Bakiev Tair</i>	65
"Self-sensitization" of Photocatalytic Activity of ZnO into visible region for $CO + NO \xrightarrow{h\nu} CO_2 + 1/2 N_2$ reaction <i>Blashkov Ilya.....</i>	66
Optical characterization of GaAs based heterostructures <i>Blinov Grigorii.....</i>	67
Magnetic-field induced variation of energy dispersion of exciton in CdTe <i>Bodnar Stanislav.....</i>	68
Defects and structure study of ferromagnetic opal-like films by GISAXS technique <i>Dubitskiy Ilya, N.A. Grigoryeva, A.A. Mistonov, I.S. Shishkin, S.V. Grigoriev</i>	69
Interpretation of Raman spectrum of cyclic clusters $(ZnO)_n$ within the polarizable bond model <i>Dymnikova Daria.....</i>	70
Structural stability of $(Ba_{0.5}Sr_{0.5})(Co_{0.8}Fe_{0.2})_{1-x}Nb_xO_{3-\delta}$ at intermediate temperature depending on the Nb concentration <i>Egorova Yulia.....</i>	71

Synthesis and the electronic structure of graphene on the cobalt surface <i>Erofeevskaya Anna</i>	72
NEXAFS study of mixed ionic electronic conducting perovskite Sr(Fe,Ti)O ₃ <i>Galdina Kristina, Egorova Yulia</i>	73
Formation of Mn/Si interface and its magnetic properties <i>Grebenyuk Georgy</i>	74
Direct numerical solution of Schrödinger equation for excitons in quantum wells <i>Khramtsov Evgeniy, Belov Pavel, Grigoryev Philipp</i>	75
Asymmetric Thermal Lineshape Broadening in the Dimerised Antiferromagnet BaCu ₂ V ₂ O ₈ <i>Klyushina Ekaterina</i>	76
Chemical bonding of organo-silicate glasses <i>Konashuk Aleksei</i>	77
X-ray spectroscopic study of oxygen scavenging from γ -Al ₂ O ₃ -film depending on material of top electrode and its annealing <i>Konyushenko Marina, Konashuk Aleksei</i>	78
Embedding potential method in electronic structure and X-Ray emission bands calculations of MgO clusters <i>Milov Igor</i>	79
Central peak of electromagnetic radiation from corrugated graphene <i>Mukhamadiarov Ruslan</i>	80
Beyond one-electron model of X-Ray band emission: Ti metal <i>Nikiforov Sergey, Ovcharenko Roman</i>	81
Theoretical investigation of manifestations of polar optical phonons in Raman spectra of short-period strained GaN/AlN superlattices <i>Pankin Dmitrii</i>	82
Magnetic anisotropy of ultrathin Fe films on the SiO ₂ /Si (111) surface <i>Pavlov Alexander</i>	83
Graphene synthesis by segregation of carbon atoms through the Ni film <i>Pudikov Dmitrii, Zhizhin Evgeny</i>	84

Synthesis of graphene by decarbidization of Gd <i>Shevelev Victor</i>	85
Bleaching effect in resonant reflection spectra from single GaAs/AlGaAs quantum wells <i>Solovev Ivan</i>	86
Modification of the electronic and spin structure of topological insulators by noble metals intercalation <i>Sostina Daria</i>	87
Study of magnetic structure of compound $Mn_{0.75}Fe_{0.25}Ge$ by small-angle neutron scattering <i>Sukhanov Alexander</i>	88
Structure and Stability of WC Nanorods <i>Teil Vitaliy</i>	89
Formation and electronic structure of graphene on cobalt silicide <i>Vopilov Anton</i>	90
Features of the electronic structure of graphene on SiC with intercalated atoms of Pt <i>Voroshnin Vladimir</i>	91
A complex study of copper-exchanged mordenites by XRD, XPS and ICP methods <i>Zhukov Yuri</i>	92
F. Optics and Spectroscopy	93
Modeling of the argon metastable radial profile in discharge plasma <i>Butris Mariia</i>	94
Dipole moments of the $I_2(G1_g \rightarrow 1_u(ab))$ transitions and spectroscopic characteristics of the $1_u(ab)$ states <i>Cherepanov Igor</i>	95
Coherent interaction of a femtosecond laser with a dense resonant medium of atomic rubidium vapor <i>Elmurzaev Ruslan</i>	96

Study of rovibrational absorption spectra of CH ₃ CN... HF complexes in the gas phase <i>Glazachev Evgenii</i>	97
H ₂ O...HF hydrogen bonded complex. Effect of H/D substitution on libration of H ₂ O and stretching motion of HF <i>Gornovesov Aleksei</i>	98
Spectral dependence of photoinduced hydrophilicity of ZnO nanofilms <i>Grishina Anastasia</i>	99
Four wave mixing and computer simulation of nonlinear optical interactions <i>Kiselev Fedor kisteddy@gmail.com</i>	100
Theoretical investigation of Raman spectra of tubular ZnO nanoclusters <i>Kizirov Eskendir</i>	101
Y ₃ Al ₅ O ₁₂ :Eu ³⁺ nanoparticles as luminescent markers for biology and medicine <i>Kolesnikov Ilya, D. Tolstikova, A. Povolotskiy, A. Manshina, M. Mikhailov</i> ..	102
Correlated librations of HCN and HF monomers in the HCN...HF hydrogen bonded complex <i>Koshevarnikov Alexey</i>	103
Spectral-luminescent study of polycrystalline phenanthrene <i>Kushaeva Mata</i>	104
Distortion of IR spectra caused by reflection <i>Murzin Petr, Novikov Roman</i>	105
Verification of current data and line assignments in vibro-rotational structure of the i ³ Π _g [±] → c ³ Π _u [±] band system of the H ₂ molecule <i>Nemchaninov Alexandr, Mikhailov A.S.</i>	106
Aggregation of molecules of mefenamic, niflumic and N-phenylanthranilic acid in dichloromethane solutions at various concentrations <i>Nosova Daria</i>	107
Multiphoton ionization of rare gas from ground and metastable states <i>Pavlov Kirill</i>	108
NEXAFS study of composite MWCNT/(pyrolytic Cr) <i>Petrova Olga</i>	109

Plutonium speciation in aqueous solution studied by Pu L ₃ and M ₅ edge high energy resolution XANES technique <i>Pidchenko Ivan</i>	110
Excited state dynamics of substituted tetraphenylporphyrin-fullerene dyads <i>Pyshnyak Marina</i>	111
Four-wave coherent interaction of the femtosecond laser pulses with Rb vapour <i>Semykina Valeriya</i>	112
Effect of F-doping on the photocatalytic activity of titania <i>Shaitanov Leonid</i>	113
Confocal ring cavity <i>Shalymov Yegor</i>	114
Kerr effect and short-range order in mesogenic compound melts <i>Shevliagin Arsenii</i>	115
Adaptive optics testing at the long-distance in-door atmosphere path <i>Shubenkova Elena, Gorelaya Alina</i>	116
Study of the ‘memory effect’ at breakdown in argon-nitrogen mixture <i>Sushentsev Danil</i>	117
Ab initio study of C—H···X hydrogen bonds along the proton transfer pathway: structure and NMR parameters <i>Tupikina Elena</i>	118
Formation and researching of silver nanoparticles in phosphate glass <i>Vasileva Anna</i>	119
Digital holographic Michelson interferometer for nanometrology <i>D.V. Venediktov¹, A.A. Sevrygin¹, I.M. Tursunov¹, O.V. Volkov²</i>	120
Observation of the difference in shape of profile for lines coming to vibrational levels of the c ³ Π _u ⁺ and c ³ Π _u ⁻ electronic states of D ₂ molecule <i>Zhukov Alexey, Umrikhin I.S.</i>	121
G. Theoretical, Mathematical and Computational Physics	123
Structural properties of thermoplastic polyimides in CNT-reinforced nanocomposites <i>Glova Artem, Serebryakov Evgenij, Larin Sergey, Lyulin Sergey</i>	124

Solution of the time-dependent Dirac equation for a hydrogenlike ion exposed to a strong laser field <i>Ivanova Irina</i>	125
Special splints and their types <i>Kakin Polina</i>	126
On the first order phase transitions in a large spin Fermi system <i>Kalagov Georgii</i>	127
Holographic estimates of the deconfinement temperature from the axial vector sector <i>Katanaeva Alisa</i>	128
Anomalous scaling of passive scalar fields advected by the Navier-Stokes velocity ensemble: Effects of strong compressibility and large-scale anisotropy <i>Kostenko Mariia</i>	129
Constraint algebra for embedding theory with partial gauge fixing <i>Semenova Elizaveta</i>	130
Influence of radial flow fluctuations on mean transverse momentum correlations in AA collisions <i>Sokolskii Vladimir</i>	131
Dynamics of triple asteroids <i>Timoshenko Vladimir</i>	132
Sensitivity of Tunneling-Rotational Transitions in Ethylene Glycol to Variation of Electron-to-Proton Mass Ratio <i>Viatkina Anna</i>	133
H. Biophysics	135
Preparation of Nanoparticles by the Reduction of Silver Ions in a Solution <i>Dokshokova Lolita</i>	136
Excited electronic states of DNA\RNA dimers: an <i>ab initio</i> study <i>Maksimov Dmitry</i>	137
DNA Fixation on Phenanthroline-Modified Gold Substrate <i>Nikolaev Dmitrii, Osolodkov Mikhail</i>	138

Electro-optical method to study aggregation in aqueous suspensions of SPIONs and SPIONs conjugated with Hsp70 <i>Parr Marina</i>	139
IR-investigation of DNA films <i>Shulenina Olga</i>	140
Estimation of photophysical parameters of silver clusters on the cytosine-containing oligonucleotide <i>Sych Tomash, Volkov Ivan</i>	141
Thermodynamics of the interaction of DNA molecule with papaverine analogue containing indole substitute <i>Travkina Veronica, Osinnikova Daria</i>	142
I. Resonance Phenomena in Condensed Matter	143
Self assembly processes of biodegradable surfactants as studied by NMR <i>Dmitriev Roman</i>	144
Concentration effect on ^7Li quadrupolar relaxation in LiCl aqueous solutions: a molecular dynamics simulation study <i>Egorova Mariia</i>	145
Principles of dynamic nuclear polarization in a low magnetic field <i>Furman Dmitry</i>	146
Diffusion NMR imaging in magnetic field 7 mT <i>Ievleva Svetlana, Luzhetckaia Nadezhda</i>	147
A magnetic field mapping for MRI scanner at 7 mT <i>Ivanov Viacheslav</i>	148
The hydration layer around the B1 domain of immunoglobulin-binding protein L and water proton magnetic relaxation. A molecular dynamics simulation study <i>Krylova Ekaterina</i>	149
NMR measurement of selfdiffusion in low magnetic field <i>Luzhetckaia Nadezhda, Ievleva Svetlana</i>	150
Magnetic resonance study of atomic hydrogen and deuterium stabilized in solid H_2 and D_2 matrices below 1K <i>Sheludiakov Sergey</i>	151

Hydrogen self-diffusion processes in the lattice of transitional metal alloys <i>Iyvodtceva Anna, Bavrina Olga</i>	152
Nuclear polarization and relaxation in Si:P at ultra-low temperatures <i>Zvezdov Denis</i>	153
S. First Steps in Science	155
DNA complexes with coordination compounds containing phthalocyanines and their stability in water solution <i>Dyachkova Olga</i>	156
Optical spectra of excitons in high-quality quantum well <i>Makarova Oksana</i>	157
The study of three-component complex (DNA, surfactant, phthalocyanine) stability <i>in vitro</i> <i>Riazantseva Valentina</i>	158
IR study of ozone adsorbed on CaF ₂ <i>Sivokhina Maria, Belykh Roman</i>	159
Ionocraft – high voltage capacitor <i>Sviridov Alexander</i>	160
DNA absorption spectra in complexes with anticancer drugs cisplatin, carboplatin, and a novel compound BP- C1 <i>Vergasova Ekatherina</i>	161

