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Dedicated to the 100th anniversary
of the National Academy of Sciences of Ukraine

SPECTROSCOPY OF MOLECULES AND CRYSTALS

Book of Abstracts
of XXIII Galyna Puchkovska International School-Seminar

(Kyiv, Ukraine, September 20–25, 2017)

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The Book contains abstracts of reports presented at XXIII Galyna Puchkovska International School-Seminar “Spectroscopy of Molecules and Crystals” dedicated to the 100th anniversary of the National Academy of Sciences of Ukraine (20-25 September, 2017, Kyiv, Ukraine). The abstracts cover recent advances in theoretical and experimental spectroscopy of crystalline and amorphous solids, liquid crystals, biological objects and polymers, nanosystems, thin films, surface and intermolecular interactions. Non-linear optical phenomena, computer simulation, as well as up-to-date spectroscopic methods and instrumentation are included.

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В збірнику представлені тези доповідей XXIII Міжнародної Школи-семінару імені Галини Пучковської “Спектроскопія молекул і кристалів”, присвяченій 100-річчю Національної академії наук України (20-25 вересня 2017 р., Київ, Україна). В тезах викладено нові результати досліджень з основних напрямків сучасної теоретичної і експериментальної спектроскопії неметалічних кристалів, аморфних речовин, рідких кристалів, полімерів і біологічних об‘єктів, нанорозмірних систем, тонких плівок, поверхні і міжмолекулярної взаємодії. Також розглянуто такі напрямки як нелінійно-оптичні явища, комп‘ютерне моделювання, нові прилади та методи спектральних досліджень.

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Dear Participants

of XXIII Galyna Puchkovska International School-Seminar
“Spectroscopy of Molecules and Crystals”
dedicated to the 100th anniversary
of the National Academy of Sciences of Ukraine,

With a great pleasure I welcome you all in the city of Kyiv - the historical, cultural and scientific centre of Ukraine. On behalf of the Organizing Committee of XXIII ISSSMC, I thank you for participating in this scientific forum and wish you fruitful creative work during extensive discussions on topical issues of spectroscopy.

Launched in 1973, this scientific forum is held every two years in different places of Ukraine covering almost all its major research and educational centres, such as Lviv, Kharkiv, Odessa, Chernovtsy, Lutsk, Sumy, Poltava, Sevastopol, Ternopil, and others. While the National Academy of Sciences of Ukraine is marching to its century anniversary in the next year, we decided to move the XXIII Galyna Puchkovska International School-Seminar “Spectroscopy of Molecules and Crystals” to the city of Kyiv, the heart of Ukrainian science.

Aiming to broaden the involvement of young researchers and to extend application of spectroscopic methods into the various branches of science and industry, to exchange the latest advances, Galyna Puchkovska International School-Seminar “Spectroscopy of Molecules and Crystals” became an indicator of scientific activity in different fields of spectroscopy and practical application of spectroscopic methods in industry and technology, a place for knowledge and experience sharing and new concepts formation. Direct communication between the participants of different generations from various countries opens new horizons for scientific cooperation, provides for instrumentation and infrastructure exchange, and promotes new interesting common projects.

No one could underestimate contribution of Galyna Puchkovska School-Seminar to scientific achievements of National Academy of Sciences of Ukraine and their international recognition. Among the founders of ISSSMC and the first its chairmen were academician Oleksandr Davydov, a famous scientist with the world-name, the author of the molecular excitons theory, academician Marat Shpak, the former director of the Institute of Physics of NASU, the founder of its Photoactivity Department known for its pioneer works on lasers and laser spectroscopy, academician Mykhailo Brodyn, a head of Non-linear Optics Department at the Institute of Physics, leader of non-linear spectroscopy research in Ukraine. Many former young participants of ISSSMC are now holding leading positions in Ukrainian science and education and their scientific achievements are highly recognized worldwide.

In the next 2018, the National Academy of Sciences will celebrate its 100th anniversary. It was in Kyiv, on November 27, 1918, where the constituent general meeting of the Ukrainian Academy of Sciences took place. At this meeting, Vladimir Vernadsky, geochemist with the world-name was elected as its first president. For the whole century of its history, Ukrainian Academy of Sciences has successfully completed its main mission – to carry out fundamental research, which formed the basis of successive practical applications. All this was despite the losses of World Wars I and II, the Stalinist terror, the conditions of the Cold War and the "Iron Curtain" and the chronic underfunding of recent decades. The current president of the National Academy of Science, Borys Paton, holds this position since 1962, while earlier the Academy was headed by V.I. Vernadsky (1918-1919), O.I. Levytsky (1919-1922), V.I. Lipsky (1922-1928), D.K. Zabolotny (1928-1929), O.O. Bogomolets (1930-1946), and O.V. Palladin (1946-1962) - all of them scientists with world-names.

According to the list of developments that enriched civilization, Ukrainian science stands at the forefront of the advanced countries of the world. The National Academy of Sciences of Ukraine is known to the world with its fundamental and applied research in material science and engineering, computer science, medical and biological research, as well as new aircraft and space technologies. It has given the world the first electric welding technology of metals, which was further developed into the welding of living tissues, as well as welding in open cosmic space; the first electronic computer; a system of surgical treatment of the heart and the eye; the aircraft building and space technology, - and this is not an exhaustive list. Under the leadership of academician V.M. Glushkov, the first small computer was created based on entirely new idea of the computational process and architecture, which was then developed and widely used in almost all foreign computers, unfortunately, abroad, not in Ukraine. There are also the achievements of astronomical science - the study of dwarf blue galaxies, which allow us to understand how the universe was formed. In part, these studies laid the foundation for the creation of the Large Hadron Collider, the world's largest particle accelerator, built for the CERN accelerator complex.

Modern strategic trends in the development of the world economy are inevitably associated with the latest advances in science. Thus, Ukrainian science should continue to further exist and to develop those areas in which significant achievements are already made focusing on urgent national problems.

I hope that XXIII ISSSMC will help to join your efforts for strengthening of international scientific cooperation and development of new effective devices and technologies for the benefit of the economies of all our countries.

Wishing you a successive work at the XXIII ISSSMC conference,

On behalf of the Organizing Committee

Valeriy Pogorelov

Honored Worker of Education of Ukraine,

Professor of Taras Shevchenko National University of Kyiv

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Lectures

Probing Brønsted Acidity of Protonic Zeolites with Variable Temperature Infrared Spectroscopy

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Zeolites containing the structural unit [Si(OH)Al] find wide industrial application as solid-acid catalysts in petrochemistry, biomass upgrade and the production of fine chemicals. The strength of their catalytically active Brønsted acid sites (bridging hydroxyls) is a major factor determining the catalytic performance of protonic zeolites, hence a reliable method to evaluate relative acidity is needed. Because of simplicity, IR spectroscopy of an adsorbed weak base that interacts with hydroxyl groups *via* hydrogen bonding, is often used to address the acidity of zeolites; and carbon monoxide is an archetypal probe molecule for such a purpose. The H-bonded species ZO-H···CO (where Z is the zeolite framework) can easily be monitored by IR spectroscopy at a low temperature, as hydrogen bonding brings about a red shift, Δν(OH), in the O–H stretching frequency (see Fig. 1A). The size of such a shift (assumed to correlate with the corresponding interaction energy) is frequently used to rank the Brønsted acidity of protonic zeolites. Nevertheless, recent research work [1] has revealed that correlation between ΔH^0 (the enthalpy change involved in hydrogen bonding) and Δν(OH) not always follows a general trend, as shown in Fig. 1B for the zeolites having the MWW structure type; thus, casting some doubt on indiscriminate use of Δν(OH) to rank zeolite acidity. Noteworthy, results shown in Fig. 1B were obtained by means of variable-temperature infrared (VTIR) spectroscopy, a technique that leads to simultaneous determination of the spectroscopic signature of the H-bonded complex, and the corresponding values of Δν(OH) and ΔH^0; and which thus has a clear edge over classical IR spectroscopy at a fixed temperature.

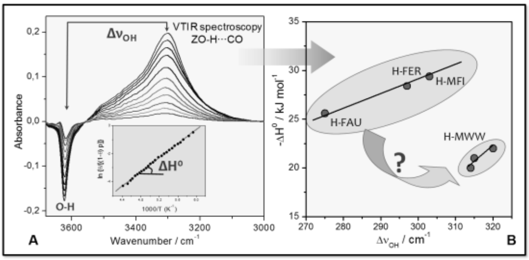

Fig. 1. A, Δν(OH) for the H-bonded CO adsorption complex in a protonic zeolite. B, correlation between Δν(OH) and ΔH^0 for several H-zeolites.

[1]. C. O. Arean et al., Phys. Chem. Chem. Phys. 2014, 16, 10129.

Ergodicity of Spin Systems and Perfectness of Nano-Structured Materials

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CP MAS is a powerful tool to determine the spatial distribution of coupled nuclei as well as to monitor the molecular mobility in solids via the spin polarization transfer rates [1,2].The CP kinetics exhibiting oscillations of intensity in the short contact time range are often observed for a broad set of materials, those as highly regular and disordered crystals as well as nano-structured compounds [2 and Refs cited therein]. Such behavior of CP intensity $I(t)$can be described in the frame of so called I–I*–S model

$$I(t) = I_0 e^{-\frac{t}{T_{1\rho}}}\left[1 - \lambda e^{-\frac{t}{T_{dif}}} - (1-\lambda) e^{-\frac{3t}{2T_{dif}}} e^{-\frac{t^2}{2T_2^2}}\right], \tag{1}$$

where $T_{1\rho}$ is the spin-lattice relaxation time of spin I in the rotating frame, T_{dif} is the spin-diffusion time constant and λ is the parameter, which describes the distribution of polarization in the S–I_N spin cluster:

$$\lambda = \frac{N-1}{2N}. \tag{2}$$

It is obvious that λ cannot overstep $\lambda \leq 1/2$. It provides an additional constraint on the processing of CP kinetic curves. Namely, the results of the non-linear curve fitting of the model and experimental data have to be rejected or revised if the minimization routine leads to $\lambda > 1/2$. In this case, the spin system exhibit non-ergodic behavior and thus the possible physical reasons, why the spin quasi-equilibrium was not reached, should be carefully analyzed.

Non-ergodic behavior of ^{31}P–^{1}H spin systems was observed in the series of nanostructured calcium hydroxyapatites containing short-range irregularities and the amorphous phase as contaminants.

[1]. V. Klimavicius, L. Dagys, V. Balevicius. Subnanoscale Order and Spin Diffusion in Complex Solids through the Processing of Cross-Polarization Kinetics.// Journal of Physical Chemistry C. – 2016. – V. 120. – N. 1. – p. 35421 – 3549.

[2]. V. Klimavicius, L. Dagys, V. Chizhik, V. Balevicius. CP MAS Kinetics Study of Ionic Liquids Confined in Mesoporous Silica: Convergence of Non-Classical and Classical Spin Coupling Models.// Applied Magnetic Resonance. – 2017. – DOI: 10.1007/s00723-017-0891-z.

Ultrashort light pulses in transparent solids: propagation peculiarities and practical applications

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In this paper we present an overview of the various techniques developed for the investigation of ultra-fast optical and electronic processes in optical materials (sapphire, quartz, semiconductor chalcohalide glasses) that are promising candidates for practical applications in optoelectronic and telecommunication devices. In particular, the main aspects of time-resolved femtosecond optical polarigraphy, femtosecond optical Kerr gate spectroscopy for time-resolved (~300fs) secondary radiation measurements, as well as Z-scan technique for probing the second-order optical non-linearity are briefly considered. The experimental observations obtained so far with the above techniques are reported, such as the formation and propagation of laser femtosecond filaments -specific physical objects of a mixed plasma-field nature, physical aspects of conelike waves generation, the filaments Superluminal moving, the femtosecond quasi-white supercontinuum generation. The examples of the femtosecond laser pulses application in practical microoptics basic components for telecommunication systems and devices such as microlens arrays, light distributors, etc., are discussed.

Two-Photon Absorbing Star-Shaped Squaraine Derivative: Linear Photophysics And Femtosecond Nonlinear Spectroscopy

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Comprehensive linear photophysical and photochemical investigations, two-photon absorption (2PA) efficiency, ultrafast relaxation processes, gain and superluminescence phenomena of new symmetrical star-shaped squaraine derivative (**1**) in liquid solutions are reported. The steady-state spectroscopic parameters of **1** in a number of organic solvents with different polarity, including excitation anisotropy spectra in low and high viscosity liquid media, revealed a weak interaction between the squaraine arms and the effect of symmetry breaking in the ground electronic state. The degenerate 2PA spectrum of **1** was investigated in a broad spectral range by open aperture Z-scan methodology, and the value of maximum cross section ~ 8000 GM was obtained. The nature of the fast kinetic processes in the ground and excited electronic states of **1** was revealed using the femtosecond transient absorption pump-probe technique, and characteristic relaxation times of 3-4 ps were shown. The efficient superluminescence properties of **1** were demosntrated under femtosecond transverse pumping in relatively low concentrated solution ($\approx 2\cdot 10^{-4}$ M). High photochemical stability, large 2PA cross sections and efficient superluminescence properties determine the potential of new star-shaped squaraine for applications in laser scanning fluorescence microscopy.

Excitons in J-aggregates of Cyanine Dyes: Photophysics and Design of Ultra-Bright and Wavelength-Converting Nanocomposites

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J-aggregates are fascinating fluorescent nanomaterials formed by assembly of organic dyes with spectroscopic properties dramatically different from that of single or disorderly assembled dye molecules. They demonstrate very narrow red-shifted absorption and emission bands, very small Stokes shifts, strongly increased absorbance together with the decrease of radiative lifetime, polarized emission and other valuable features. The mechanisms of their electronic transitions are understood by formation of delocalized excitons already on the level of several coupled monomers. Cyanine dyes are unique in forming J-aggregates over the broad spectral range, from blue to near-IR. In our work, they are stabilized by cationic polymer and are also included into a shell of nanoscale composites. Being very efficient light absorbers and converters, they offer bright prospects in different applications, particularly in live cell imaging and sensing. We demonstrate design and application in fluorescence microscopy of different nanostructures based on J-aggregates: (1). The ultra-bright wavelength-converting nanoparticles. (2). The nanoparticles for two-photon microscopy. (3). The near-IR excited nanocomposites that involve up-converting nanocrystals.

Effects and Mechanisms of Graphene Enhancement Raman Scattering (GERS)

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Graphene attracts a great interest due to their unique physical properties. One of the topics actively discussed in literature is an enhancement of optical signals from molecules absorbed on graphene surface. Here we present and discussed numerous our experiments on SERS and CARS of molecules on graphene as substrate and their comparison with literature data.

We thank for financial support to: STCU №6175, 690853-assymcurv-H2020-MSCA-RISE-2015/H2020-MSCA-RISE-201 and Ukrainian-Poland project 2015-2017 years.

Spectral Methods Used in Characterizing the Excited Electronic States of Molecules

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For the molecules showing absorption and fluorescence spectra, there are studies in which the excited state dipole moment and the angle between the dipole moments in the ground and excited states are estimated when the dipole moment of the ground electronic state was experimentally determined or it was computed using quantum chemistry methods.

Some information about the excited state parameters of non-fluorescent molecules can be obtained from the absorption spectra. The solvatochromic analysis offers the possibility to characterize the molecule in its excited state when the contribution of the universal interactions to the spectral shifts is higher than the contribution of the specific interactions. The theory of simple liquids applied to the diluted solutions of the spectrally active molecules express the contribution of universal interactions as function of the solvent macroscopic parameters and of the solute microscopic parameters in its electronic states participating in absorption process.

The results regarding the characterization of some azo-dyes are discussed here, by combining the quantum mechanical analysis and the solvatochromic study.

Monitoring and Quantification of Engineered Nanomaterials at Single Cell Level by Means of Element-and Molecule Based Imaging and Dosimetric Techniques

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Increasing applications of engineered nanomaterials (ENMs) in the industry and private consumption demand the thoroughly identification of hazards and potential adverse effects on human and environment. These adverse effects include the ability of ENM to induce damage at the cellular, tissue, or organism levels by interacting with cellular structures. Modifying the surface chemistry of nanomaterials has been used to understand and control the potentially toxic impact of nanomaterials, their translocation and localization.

The translocation of ENMs across plasma membranes was studied in cancer culture cells *in vitro* as well in lung tissues of exposed rats *in vivo* by means of label-free imaging methods based on elemental and molecule analysis. Proton induced X-ray emission (µPIXE) and Rutherford backscattering (µRBS) were used simultaneously at the Leipzig Ion Nanoprobe LIPSION for cell analysis. These two IBM techniques provide unique and powerful tools for element dosimetry and spatially resolved elemental analysis. The results of ENM uptake *in vitro* were compared with *in vivo* study providing a tool for estimating the relevance of in vitro data for in vivo predictions.A quantitative analysis of minor and trace elements and their alterations due to NP loading at single cell level were performed and correlated with the cellular adverse response. Ion Beam analysis revealed an influence of ENMs on the homeostasis of certain elements, like iron, copper or zinc. It was found that the cellular uptake of ENMs was strongly influenced by their surface properties and formation of biocorona in extracellular space. The dynamics of the ENM-biocorona was monitored. The post-modifications of the NM surface in biological matrixes were supposed to have a significant impact on the characteristics of the cellular uptake and as consequence on the toxicological response of bio-systems to ENM exposure. Furthermore, ENM subcellular localization and co-localization with cell compartments and biomolecules were investigated using confocal Raman microspectroscopy (CRM). CRM live imaging was additionally performed to follow the intracellular fate of nanoparticles.

Nonlinear Optical Diagnostics of Porous Carbon Materials

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The response of the dielectric and semiconducting carbon materials to the electric fields of an intense laser light one can study in the paradigm of a nonlinear optic (NLO). NLO effects are rather sensitive to surface tailoring and intrinsic structural changes of the surface and near-surface layer of bulk nanoporous carbons [1]. Typically, the response measurements can found the fundamental scientific and technological applications. The measurements have a high accuracy and reasonable sensitivity; consequently, such remote diagnostic can be used for today's metrology needs. Recently, a significant progress in NLO studies directed to the most interesting family of ultra-small and dispersed carbon particles [2]. Totally diverse NLO characteristic of carbon semiconductors gave carte blanche to include this technique into an analytical kit to be used for the carbon surface interface parametrizing. Despite the mentioned facts, scanty NLO response studies were provided for bulk solid carbons, e.g. for μm and nm sized particles. However, it is a quite attractive to expand this nondestructive approach on the modern advanced composites and optical-limiting carbon materials. Also, a special attention could be paid on observing the surface functionalization effects within the use of a laser pulse self-action effects [3]. In this way, we consider the applying the diagnostic to the oxidized and fresh untreated surfaces layers of nanoporous carbons, as the model objects, for their comparative assessment. If consider the method extra sensitivity to the intrinsic defects in the solid state, the changes that are caused the surface layer oxidation could be visualized with the NLO response measurements by a single beam technique. Therefore, here we report the main results obtained at the porous μm sized particles characterization.

[1]. V. Multian *et al.* Surface response of brominated carbon media on laser and thermal excitation: optical and thermal analysis study // Nanoscale Research Letters. – 2017. – V. 12. – N. 1. – p. 146.

[2]. N. Yang, X. Jiang, D.-W. Pang (Eds) Carbon Nanoparticles and Nanostructures // Springer. – 2016. – Cham, Switzerland. – 360 p.

[3]. A. Uklein *et al.* Characterization of oxidized carbon materials with photoinduced absorption response // Applied Physics B. Letters. – 2016. – V. 122. – N. 12. – p. 287.

Electronic Structure Evolution with Pressure in Narrow Band Gap Oxides and Chalcogenides

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The desire to control magnetism with external perturbations other than magnetic fields has motivated much recent research on the pressure and strain response of magnetic materials. However, the obtained experimental results cannot be satisfactory described within existing phenomenological models. Using density-functional theory, we investigate the effect of pressure on the electronic structure and magnetic properties of representative narrow-gap semiconductors. There are perovskite-like oxides, $BiFeO_3$ and $LaCoO_3$, and also the SmS compound in the semiconducting "black" phase. It is established that these systems possess peculiar electronic structure features, which can explain their puzzling magnetic and spectral properties. Based upon these findings, we suggest that these unusual properies could originate from the band electronic states, separated by the small energy gap. Since these gaps are extremely sensitive to external pressures, a sizable piezomagnetic effect can be achieved, which could lead to practical applications in corresponding magnetopiezoelectric devices.

Exciton Dynamics in an Energy Up-Converting Solid State System Based on Diphenylanthracene Doped with Platinum Octaethylporphyrin

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Photophysics of composite solid films based on 9,10-diphenylanthracene (DPA) doped with Pt(II)octaethylporphyrin (PtOEP) have been investigated by ultrafast transient absorption and luminescence spectroscopy, as well as by nanosecond time-gated luminescence techniques. The DPA:PtOEP host:guest system is a benchmark for incoherent energy up-conversion via triplet fusion in solution and we focus here on study of the photophysical processes of this system in solid state thin films. Measurements of the kinetics of the triplet energy transfer from PtOEP to DPA show that it is a slow process taking up to tens of ns, featuring a thermally activated behavior. This implies that before triplets are transferred to the host, they migrate within PtOEP aggregates to the interface with DPA, defining a rate limiting step for the overall energy transfer to DPA. In contrast to other porphyrin-based sensitizers, no significant triplet-triplet annihilation is found to happen at the stage of triplet migration within PtOEP aggregates, implying that such a triplet loss mechanism does not universally apply to porphyrine-based organometallic complexes.

This research was supported by the ERC via Grant No. 320680 (EPOS CRYSTALLI) and by the VW Foundation through the project "Understanding the dependence of charge transport on morphology in organic semiconductor films."

Anisometric Nanoparticles in Liquid Crystals: Experimental Evidencing of Short-Range Ordering Features

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Liquid crystal (LC) dispersions of various micro- and nanoparticles (often designated as “liquid crystal colloids”) are highly topical both as objects of fundamental studies and promising materials for applications. Among the most challenging are LC systems where dispersed particles are of strong geometrical anisometry, with nanoscale sizes in one or two dimensions. As typical examples, one could note carbon nanotubes or exfoliated platelets of organoclays. In this report, we present a general review of such systems, with special accent on our recent studies in this direction.

From the standpoint of physics, the main problem is to describe incorporation of the nanoparticles into LC ordering in different matrices on the level of molecular models, accounting for inter-particle aggregation processes. The required basic information can be obtained from analysis of microphotographs, dependences of optical transmission on nanoparticle concentration, as well as data of DSC, SAXS and other studies. Among the most important results, one could note:

- accumulation of carbon nanotubes (CNT) on structural defects in cholesterics, with increased CNT concentration leading to disappearance of oily steaks and formation of inter-particle aggregates; optimum conditions can be determined ensuring high homogeneity and time stability;
- substantially different behavior with laponite platelets, with homogeneity and other characteristics depending on the degree of exfoliation, which could be controlled by varying the preparation procedures;
- stabilizing effects in mixed dispersions of particles with different anisometry;
- possibilities of novel photo-electro-optical effects in LC cells, with the planar to homeotropic transition recorded, in the presence of carbon nanotubes, by sharp jumps in electric conductivity.

Possible practical applications of the observed effects and LC-based nanomaterials are discussed.

Lyotropic Chromonic Liquid Crystals: from Molecules to Crystal

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The Lyotropic Chromonic Liquid Crystals (LCLC) family embraces a wide range of dyes, drugs, nucleic acids, antibiotics, carcinogens, and anti-cancer agents; the anti-asthmatic drug, disodium cromoglycate (known under the trade name INTAL) is one example. The LCLC are fundamentally different from the better known amphiphilic lyotropic and thermotropic LCs. Qualitatively, the LCLC molecules are plank-like rather than rod-like, rigid rather than flexible, aromatic rather than aliphatic. Theπ-π interaction of the aromatic cores is the main mechanism of molecular face-to-face stacking. Hydrophilic ionic groups at the periphery of the molecules make the material water-soluble. These distinctions create a whole new range of ordered structures. The current report highlights the physical picture of nano- and micro-scale ordering in these systems and experimental methods of its characterization. The basic principles of how the LCLC molecules aggregate, what is the structure of aggregates and how these aggregates build the phases with orientational order will be explore. Considerable effort will be focused on the interlay between molecular architecture, molecular order and macroscopic properties. An integrated approach, ranging from synthesis, purification and characterization of individual substances to development of technologies for the most effective use of optical properties of LCLC will be pursued. An integrated approach, ranging from characterization of individual substances to development of technologies for the most effective use of of LCLC materials will be pursued.

The Tragic Scrolls of Ukrainian Science. To the 100th Anniversary of the National Academy of Sciences of Ukraine

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The lecture covers the history of Ukrainian science at the turn of XIX and XX centuries, and contains several essays about prominent intellectual elite of Ukraine of that time – physicists, mathematicians, natural researchers, chemists, biophysicists, physicians, - whose outstanding scientific achievements could have been pride of any nation but who were unlawfully convicted and sent to prison or concentration camps or executed by the communist regime under the guise of the slogan “the struggle against Ukrainian bourgeois nationalism”. A life story of both the well-known and the forgotten names is unveiled under the total motto “Let the light of science never die”.

Raman Spectroscopy of Crystals and Films of Semiconducting Multicomponent Chalcegenides

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The report is a review deals with the Raman investigation of crystalline four- and three-component chalcogenides. A typical example of such compounds are chalcogenides $A^1_2\ B^2C^4(S,Se)_4$ and $A^1B^3(S,Se)_2$, such for example as Cu_2ZnSnS_4 and $AgGaS_2$. Both types of these compounds are derived from classical binary semiconductors A^2B^6. In the case of copper as an element A^1 these compounds are promising photovoltaic materials, and when atoms of silver are used as element A^1 they are good nonlinear optical materials for the red and near infrared spectrum. Important is the ability to use solid solutions with replacement of related elements in cationic or anionic sublattices.

The main problems related to the use of these compounds are a large number of atoms in the unit cell, resulting in a high concentration of possible own structural defects, breach of stoichiometry, high probability of inclusions of different phases of binary compounds.

The traditional use of X-ray diffraction in the diagnostics of these structural defects are often ineffective due to proximity of diffraction scattering angles. On a number of examples in the report there are shown that in many cases the Raman scattering of light is very informative in this regard. In addition to the diagnostical problems of such compounds, in the report there are discussed a several interesting physical problems in their vibrational spectra, such as Fermi resonance, photoinduced structural transformation, and the peculiarities of the transformation of phonon spectra in mixed compounds.

Multi Fermi-Davydov Resonances in Vibration Spectra of Hydrogen Bonded Crystals

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The investigation of the vibrational spectra of hydrogen bonded systems in condensed phases is an important topic in physics, chemistry and biology. The hydrogen bonded molecular crystals are very convenient for such studies since the translation symmetry noticeably simplifies the vibrational problem as well as it helps to clarify the role of anharmonic interactions involved in the phenomenon. However, even for simple crystals with only one hydrogen bond in a unit cell, that are considered as model systems, the anharmonic effects are very important. One of them is the phenomenon of Fermi resonance (FR) between stretching and bending vibrations of the OH-bond. Besides, there are many crystals with several identical, differently oriented hydrogen bonds in a unit cell. Therefore, as the dipole moments for stretching vibrations are oriented along the H-bonds one can expect to observe the effect of splitting of Davydov (DS) bands. In addition, one can note that complex structure of absorption bands arises due to strong coupling of H-bond vibrations with lattice phonons. Mixing of all these effects, namely, FR, DS and many phonon processes, gives rise to very complicated shape of band for H-bond vibrations.

In the present report we consider the effect of these three factors on the shape of absorption band. The analytical calculations and the model numerical calculations were carried out and the comparison of theory with experimental IR absorption spectra of H- and D- adipic acid crystals in the region of their hydrogen bond vibrations was done [1-3].

[1]. A.M. Yaremko, H. Ratajczak, J. Baran, A.J. Barnes, E.V. Mozdor, B. Silvi. Theory of profiles of hydrogen bond stretching vibrations: Fermi-Davydov Resonances in hydrogen-bonded crystals // Chemical Physics. – 2004. – V. 306. – p. 57-70.

[2]. H. Ratajczak, A.J. Barnes, J. Baran, A.M. Yaremko, Z. Latajka, P. Doperalski. Anharmonic interactions and infrared band shape of the hydrogen bond vibration of potassium hydrogen (deuterium) maleate crystals // J. Molec. Structure. – 2008. – V. 887. – p. 9-19.

[3]. A.M. Yaremko, H. Ratajczak, A.J. Barnes, J. Baran, P. Durlak, Z. Latajka. Fermi resonance and strong anharmonic effects in the absorption spectra of the v-OH (v-OD) vibration of solid H- and D-benzoic acid // Chemical physics. – 2009. – 364. – p. 51-63.

2
Molecules

Phase Transitions of *Ortho*-benzylphenol and Its Crystallization Behavior

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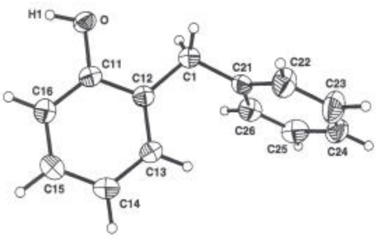
Ortho-benzylphenol is an organic material with the formula ($C_{13}H_{12}O$) that undergoes a glass transition and different polymorphic transitions and for that reason it has been the subject of several experimental studies and theoretical considerations [1-3]. Besides *ortho*-benzylphenol has application as efficient extractant for Cs^+, making it good candidate for nuclear waste cleanup.



The molecule of *ortho*-benzylphenol consists of two phenol rings that are connected by methylene bridge ($–CH_2–$) and a hydroxyl group (– OH) attached to *ortho* position of the ring. It was established that *ortho*-benzylphenol molecule can exist in four stable conformations [1]. The presence of several conformers gives rise to the observation of the corresponding number of ν_sCH_2 and $\nu_{as}CH_2$ bands in the IR spectra, thus providing experimental evidence of the conformational sensitivity of the νCH_2 frequencies. Besides they are not especially liable to intermolecular interactions and could therefore be used as a probe for conformational changes. With vibrational spectroscopy we monitor the methylene bridge vibrations νCH_2, during phase transformations. *Ortho*-benzylphenol was also studied by differential scanning calorimetry to identify the polymorphs and their most favorable formation conditions.Two metastable polymorphs were observed, with melting temperatures near 17 and 23 °C, when different formation conditions are used.

[1]. S. Katsyuba, A. Chernova, R. Schmutzler. Org. Biomol. Chem. – 2003. – V. 1. – p. 714-719.
[2]. J.J. Moura Ramos, S. Rocha, H.P. Diogo. J. Non-Cryst. Solids. – 2004. – V. 344. – p. 119-127.
[3]. J. C. Bryan, L.H. Delmau, J.B. Nicholas, L.M. Rogers, R.D. Rogers, B.A. Moyer. Structural Chemistry. – 1999. –V. 10. – N3. – p. 187-203.

Spectral Study of Model Membrane Fluidity Using a Fluorescent Marker

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Measuring the spectral characteristics of the fluorophore molecule is a method for obtaining information about the marker location in the cell membrane bilayer. As fluorescent probe is used 1,6-diphenyl-1,3,5-hexatriene (DPH) with special properties depending on the surrounding factors. The spectral modification in the electronic spectra can be correlated with the depth of DPH bounding in bilayer and the environmental factors.

The Comparison of Theoretical and Experimental Data for Guanidinium Trichloroacetate Complex

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A guanidine molecule with only ten atoms (CN_3H_6) belongs to the simplest organic chemical compound, but plays a crucial role in the features of investigated compounds. The specific planar configuration with sp^2 hybridization of carbon atom makes that investigated cation can be used as potential H-donor in hydrogen bonds and these “weak” chemical interactions play the most important role in studied compounds. On the other hand, high symmetry (D_{3h}) of investigated molecule can be used for design of new compound with using rules of supramolecular chemistry.

Ten years ago, the theoretical calculations of equilibrium geometry, vibrational spectra and potential energy distribution (PED) were performed for real guanidinium acetate complex [1]. The very good agreement between experimental and theoretical spectra was found. On the basis of this work, the theoretical DFT calculations were extended for two “virtual” complexes: guanidinium trichloroacetate and guanidinium trifluoroacetate. The obtained results (values of calculated enthalpies) suggest strongly that these two compounds should exist in real experiment.

After many attempts the guanidinium trichloroacetate compound was synthesized. The small crystals of guanidinium trichloroacetate were grown from the aqueous solution containing guanidinium cations and trichloroacetate anions in a stoichiometric ratio 1:1 at stable ambient temperature.

For this new compound, the detailed X-ray crystallographic studies were performed. Additionally, the IR and Raman spectra were measured. Unfortunately, the DSC investigations performed in the range 100 – 400 K did not show any phase transitions. These experimental results and previous DFT calculations will be presented in detail.

These shown results should give reply to the most important question: Are carried out theoretical calculations (predicted structure and vibrational spectra) compatible with received experimental results?

[1] M. Drozd, Spectrochimica Acta A 69 (2008), 1223.

Nature of the Peculiar Points for Aqueous Solutions of Alcohols

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The physical nature of peculiar points for aqueous solutions of alcohols is studied. The peculiar point is defined as the intersection points of the contraction curves. The contraction is defined as

$$\varphi = \frac{V_{12}}{V_1 + V_2} - 1,$$

where V_{12} is the volume occupied by aqueous solution of alcohol and V_1 and V_2 are initial volumes of its components ($V_{12} < V_1 + V_2$). In general, the contraction is a function of molar concentration x and temperature t and its behavior for aqueous solutions of ethanol is presented in Fig. 1.

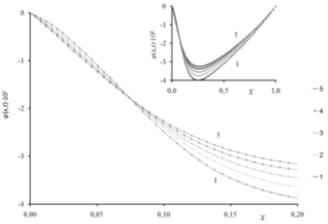

Fig. 1. Concentration dependencies for water-ethanol contractions $\varphi(x,t)$ for different temperatures t: 1 - 0°C, 2 - 10°C, 3 - 20°C, 4 - 30°C, 5 - 40°C. The vicinity of the intersection point is given in the insert

From Fig. 1 it follows that the contraction curves intersect at $x = 0.077$, i.e. namely this intersection point is the peculiar point of water-ethanol solutions. It is essentially that the contraction effect is the most expressed for water-ethanol solutions. The anomalous increase of the integral intensity for molecular light is another characteristic manifestation of the peculiar point.

This paper is devoted to the consideration of the physical nature of the peculiar points for aqueous solutions of alcohols of the methanol series. We will show that the peculiar points of water-alcohol solutions are genetically connected with the existence of the minimum for the specific volume of water at $4^0\ C$.

In our report we a) present the most characteristic manifestations of the peculiar points in different thermodynamic and kinetic processes; b) consider the role of the averaged interparticle interactions and H-bonds in the formation of characteristic properties of water and alcohols; c) show that the peculiar points in water-alcohols solutions as well as the maximum of density in water are results of specific competition of contributions caused by the averaged interparticle potentials and H-bonds; d) give the weight arguments in the favor of electrostatic nature of H-bonds.

Spectral Study of the Collective Properties of Vibrational Modes of $CHCl_3$ in Solutions with CH_3OH

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The detection of the LO-TO splitting for the strongest IR mode $\boldsymbol{\nu}_5$(E) of liquid $CHCl_3$ in the Raman scattering spectra (RS) [1] raises the general problem of studying the changes in the LO-TO splitting of $\Delta\boldsymbol{\nu}_{\mathbf{LT}}$ in fluid solutions. The forms of the vibrational bands $\boldsymbol{\nu}_\mathbf{4}$(E),$\boldsymbol{\nu}_5$(E), and also the overtones 2$\boldsymbol{\nu}_\mathbf{4}$, 2$\boldsymbol{\nu}_\mathbf{5}$ and a number of compound tones in the IR absorption spectra and RS (excitation of 710 nm) of liquid $CHCl_3$ and its solutions in CH_3OH are studied in detail. It was found that the TO and LO components of the $\boldsymbol{\nu}_5$(E) band are clearly manifested in the spectral differences, as shown in Fig. 1a. It was found that with decreasing of C, the values of $\boldsymbol{\Delta}_{\mathbf{LT}}$ decrease from 16-19 cm^{-1} to 9-10 cm^{-1}. This is due to the preservation of clots (globules) of $CHCl_3$ with expressed collective oscillation properties at C=2.5-5 vol. %. For the $\boldsymbol{\nu}_4$ IR band, weaker in comparison with $\boldsymbol{\nu}_5$, the value of $\boldsymbol{\Delta}_{\mathbf{LT}}$ is small. Therefore, the presence of the doublet band of the overtone 2$\boldsymbol{\nu}_\mathbf{4}$ in the IR and RS $CHCl_3$ spectra (see the inset in Fig. 1b) for simple lines $\boldsymbol{\nu}_\mathbf{4}$ can be associated with the manifestation in the second-order bands of vibrational states 2$\boldsymbol{\nu}_\mathbf{4}$(**k**) in the region of large wave vectors **k**. This is confirmed by the observation of additional spectral components $\boldsymbol{\nu}_\mathbf{4}$(**k**)=1235-1240 cm^{-1} in solutions, which is due to the distortion of the liquid structure and for the IR band at C = 30% is shown in another inset in Fig. 1b. Dependences on C the frequencies $\boldsymbol{\nu}_\mathbf{4}$ and $\boldsymbol{\nu}_\mathbf{4}$(**k**) in the IR spectra of solutions of $CHCl_3$ in CH_3OH are shown in Fig. 1b. The quantities $\Delta\boldsymbol{\nu}=\boldsymbol{\nu}_\mathbf{4}(\mathbf{k})-\boldsymbol{\nu}_4$ and $\mathbf{2}\boldsymbol{\nu}_\mathbf{4}(\mathbf{k})\mathbf{-2}\boldsymbol{\nu}_\mathbf{4}$ characterize the widths of the phonon bands. The developed concept is confirmed by the existence of a similar doublet structure in the bands $\boldsymbol{\nu}_\mathbf{1}+\boldsymbol{\nu}_\mathbf{4}$ and $\boldsymbol{\nu}_\mathbf{1}+\mathbf{2}\boldsymbol{\nu}_\mathbf{4}$. All the facts prove the existence of phonon branches $\boldsymbol{\nu}_\mathbf{4}(\mathbf{k})$ with a positive dispersion d$\boldsymbol{\nu}_\mathbf{4}$/d**k**>0.

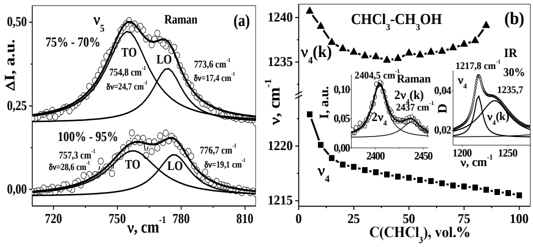

Fig. 1a,b

[1]. N.E. Kornienko., Ukr. J. Phys.- 2001. -V.46.- № 5-6.-p.546-552.

Complexation in Aqueous Solutions of Isopropanol: 2D COS and MCR Analysis of Vibrational Spectra

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Molecular complexes formation in aqueous solutions of isopropanol is investigated by ATR FTIR and Raman spectroscopy. Spectra were detected in the spectral region of stretching CH and OH vibrations for solutions with different concentrations of isopropanol and water: from pure isopropanol to pure water with concentration step of 5% (vol.).

Generalized two dimensional correlation spectroscopy (2D COS) were used for the detection of regions where spectral response varies nonlinearly with concentration changes. Such regions reflect influence of intermolecular interaction (e.g., complex formation) on measured spectra. Both 2D COS and principal component analysis of ATR FTIR and Raman spectra of isopropanol-water solutions indicate that there are at least two types of complexes in the investigate solution. Four-component MCR-ALS decomposition was performed to obtain concentration and spectral profiles of solution species. The obtained four components were identified as pure isopropanol, pure water, complex 1 and complex 2. The maximal concentration of the complex 1 is reached when isopropanol/water molar ratio equals 1:2.3. The complex 2 is dominant structure unit in the water rich region. The maximal concentration of complex 2 is reached when molar ratio of isopropanol water equals to 1:8.8. The regions where concentration of complexes is dominant correspond to concentration regions where some physical characteristics of solutions have extreme values: for example, self-diffusion coefficient [1], dielectric permittivity [1], excess enthalpy [1], terahertz absorption coefficients [2], sounds absorption coefficient [3].

[1]. R. Li et al. Mesoscopic structuring and dynamics of alcohol/water solutions probed by terahertz time-domain spectroscopy and pulsed field gradient nuclear magnetic resonance // *J. Phys. Chem. B.* – 2014. – V. 118. – P. 10156-10166.

[2]. J. McGregor et al. Structure and dynamics of aqueous 2-propanol: a THz-TDS, NMR and neutron diffraction study // *Phys. Chem. Chem. Phys.* – 2015. – V. 17. - P. 30481-304091.

[3]. L.A. Bulavin, A.V. Chalyi, and O.I. Bilous. Anomalous propagation and scattering of sound in 2-propanol water solution near its singular point // *J. Mol. Liq.* – 2017. – V. 235. – P. 24-30.

FTIR Spectra of Water in Ar Matrix and in Condensed State

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The spectral formations of hydrogen bonds between water molecules are investigated by method of matrix isolation. Also, FTIR spectra for water in condensed state were registered in temperature range from -30℃ to +50℃. Special attentions is given for investigation the behavior of water molecules at phase transition temperature liquid – solid state. The changing of spectral characteristics (band position in IR spectra, their half-width, intensity) with changing of temperature are discovered and presented in this work. The package Gaussian 03 for quantum - chemical calculations was chosen for theoretical calculations and modeling different water structures.

All presented spectra were registered in the laboratory of Fourier transform infrared absorption spectroscopy at Physics Department of Vilnius University, Lithuania. The spectra for water were recorded using Bruker's FTIR spectrometer VERTEX 70 (condensed state) and Bruker's FTIR spectrometer IFS 113(isolated in matrix) with using the thermo stabilize equipment LINKAM cryostat (model FTIR 600). The IR spectra were recorded in the spectral range from 500 to 4000 cm^{-1}.

The investigation was carried out in the frame of Ukrainian-Lithuanian bilateral agreement supported by Ministry of Education and Science of Ukraine (grant M/82-2017). The research was supported by the State Fund for Fundamental Research of Ukraine (grant Ф73/31 – 2017).

[1]. J. Ceponkus, P. Uvdal, and B. Nelander, Water Tetramer, Pentamer, and Hexamer in Inert Matrices, J. Phys. Chem. A 2012, 116, 4842−4850.
[2]. J. Ceponkus, A. Engdahl, P. Uvdal, B. Nelander, Structure and dynamics of small water clusters, trapped in inert matrices, Chemical Physics Letters 581 (2013) 1–9.
[3]. V. Pogorelov, I. Doroshenko, G. Pitsevich, V. Balevicius, V. Sablinskas, B. Krivenko, L.G.M. Pettersson, From clusters to condensed phase – FTIR studies of water. J. Mol. Liq. (2016), http://dx.doi.org/10.1016/j.molliq.2016.12.037.

Matrix Effect on the Electrooptical Properties of heptylviologen

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This work relates to studying an electrooptical behaviour of viologen molecules incorporated into different liquid and viscous matrices, namely water, lyotropic liquid crystals, aqueous solution of polyvinyl alcohol, etc. Results obtained by methods of optical spectroscopy revealed that matrix has a strong effect on absorption of viologens in the visible region, causing a significant peak shift between different host media. Since viologens absorb only being in their radical cationic or dimeric state formed under the action of electric field, this change in the absorption means that matrix may influence an electron transfer, which occurs upon voltage application. Particularly, it affects the rates of reduction processes which lead to the formation of coloured radical cations and dimers.

Cluster Structure Changes during Melting of 1-decanol: FTIR Study and DFT Calculations

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Temperature dependence of 1-decanol FTIR spectra (Fig. 1) is studied from both sides of melting point with a step of 0.5 °C near the phase transition.

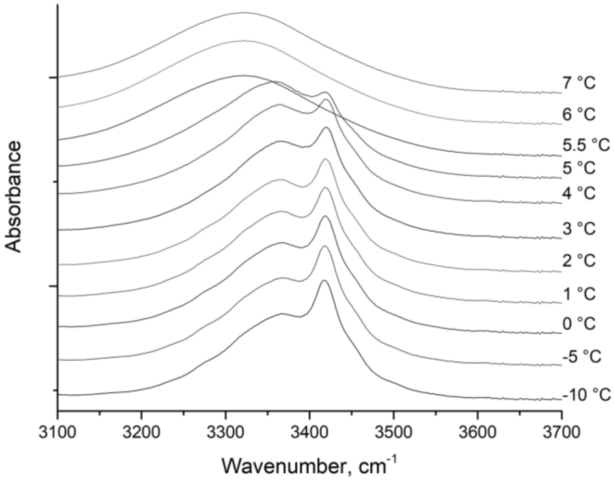

Fig. 1. Temperature evolution of FTIR spectra of 1-decanol at temperatures from -10 to +7 °C in the spectral region 3100 – 3700 cm^{-1}

Using ab initio quantum-chemistry calculations of different cluster structures, it was shown that solid phase of alcohol is formed by clusters consisting of 3 molecules and liquid phase – by clusters consisting of 5 molecules. Unlike small alcohols, 1-decanol is formed by chain-like clusters. Gradual changes of spectral bands in process of heating are interpreted as a feature of amorphous phase.

The work was carried out in the frame of Ukrainian-Lithuanian bilateral agreement supported by Ministry of Education and Science of Ukraine.

Dynamics of Vibrational Spectra and Interaction of Molecules in Liquids

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The study of the vibrations of polyatomic molecules has recently became one of the most powerful and widespread methods for investigating the structure of molecules. These oscillations appear in the spectra of Raman scattering in gases, liquids, solid materials and provide information on the structure of liquids. Investigating such oscillations gives opportunity to detect the presence of intermolecular complexes and associates in them, and to study intermolecular dynamics.

In this thesis, we present the results of investigation of the vibrational relaxation of the benzene and brombenzene molecules in the liquid state using the Raman spectrum.

The choice of the benzene molecule is due to its high symmetry, and the molecules of bromobenzene that it is a benzene ring with attached halogen groups.

The junction of halogen groups to the benzene ring in the bromobenzene molecule makes these molecules sapid objects for studying the influence of the hydrocarbon substituent on the nature of the relaxation processes of molecules in the liquid phase.

The Raman spectra were registrated using the experimental setup STR250 Laser Raman Spectrometer with a tuned confocal microscope. The 532 nm laser with a power of 50 mW was used as a radiation source.

For the Raman line related to depolarized spectra an important to have mechanism of broadening the resonance exchange of energy, i.e. the exchange of energy quanta of intermolecular vibrations between oscillators of the same type. Resonant energy exchange can make a significant contribution to the form of Raman's strips in pure liquids with sufficiently strong intermolecular interactions.

It was found that resonance energy transfer, in addition to broadening the band contours in liquids with strong intermolecular interactions of a directed character, should cause the positions of the maxima of the bands of the same vibration to mismatch in the spectrum of the polarized and depolarized Raman spectrum.

The observed patterns are discussed in the framework of existing mechanisms involving intermolecular interaction specificity.

Kinetics of Ionic Processes in Aqueous Sodium Phosphate Solutions as Studied by Broadband Acoustic Spectroscopy

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Sodium orthophosphates represent the well-known components of great variety of natural and artificial biological systems. In many cases the possibility of tuning the ionic equilibrium of sodium orthophosphates in aqueous solutions is important for their application.

In our previous work the mechanism of internal mobility of globule of human serum albumin was studied by acoustic relaxation spectroscopy [1]. The study showed that in addition to the protein conformational dynamics, the elementary processes occurring in the aqueous solution of sodium phosphate buffer contribute to acoustic relaxation of the sample. Proton transfer processes on phosphate anions are commonly believed to cause the sound absorption in such systems [2]. To shed more light on this effect a more systematic investigation of the acoustic spectra in aqueous solutions of sodium phosphates was required.

In the present work the sonic absorption spectra between 0.2 and 2000 MHz have been recorded in aqueous solutions of individual compounds H_3PO_4, NaH_2PO_4, Na_2HPO_4, and Na_3PO_4 as well as their binary mixtures in the ranges of pH from 1.8 to 12.3, concentrations from 0.1 to 0.3 mol/l, and at 288 K. The spectra were approximated by analytical functions that consisted of one or two Debye-type relaxation terms depending on the composition and concentration of solution. Only two relaxation processes observed at frequencies around 500 and 20 MHz in the solutions with extreme pH 1.8 and 12.3, respectively, could be satisfactorily described by proton transfer reactions. The combination of phosphate ion hydration process with relaxation time around 0.5 ns and the process of phosphate ionic association with relaxation time around 5 ns was suggested for the most consistent description of the acoustic relaxation spectra in all solutions. Thus, contrary to common belief, all three sodium phosphate salts could show significant ion-pair formation.

[1]. T. Hushcha, A. Peytcheva and U. Kaatze. Broadband acoustic spectra of aqueous solutions of human serum albumin // J. Phys.: Condens. Matter. – 2002. - V. 14. – P. 9461-9464.

[2]. U.Kaatze, T.O.Hushcha and F.Eggers. Ultrasonic broadband spectrometry of liquids – research tool in pure and applied chemistry and chemical physics // Journal of solution chemistry. – 2000. –V. 29. – N. 4. – P. 299-368.

On the Mechanism of Formation of Anomalous Properties of Water

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Water plays an important role in various physical and biological processes, including in technological processes. It has various abnormal properties and plays a decisive role in the course of human activity. In studies, an extreme sensitivity of the structure of the water molecule to external influences is observed [1]. In the ice, 13 species of crystalline form were found. In the vapor state, exposure to ultraviolet radiation increases the length of the O-H bond and the angle between the H-O-H bonds [2]. In liquid state water is in four states and they are located in the four temperature range: 0 to 15 °C, 15 to 30 °C, 30 to 45 °C and 45 to 60 °C. Because of the extreme sensitivity of the structure of the water molecule to external influences, its structure changes in a quantized way and this leads to a quantized change in the structure of the ice.

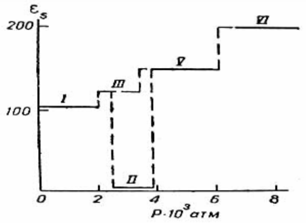

Fig. 1. Dependence of polymorphic forms of ice on pressure [1].

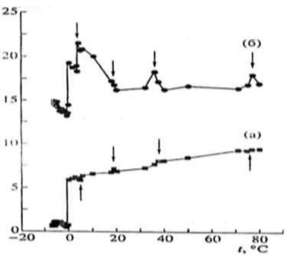

Fig. 2. Dependence of the center of the valence bond band (a) and the half-width (b) of water on temperature [3].

Despite numerous works devoted to the study of the properties of water, it is not possible to explain the cause of the formation of anomalous properties of water. The reason for the current situation in this issue is the need to take into account the field-substance interaction. According to observational data, the energy density of the surrounding physical vacuum or vacuum fluid is much higher than the energy density of the atomic nucleus [4]. Using this presentation, the reason for the formation of abnormal properties of water and the role of water in the vital activity of living systems, including man, were discussed.

[1]. N. Maeno. The science of ice - M .: Mir, 1988. -231 p.
[2]. Zatsepina G.N. Properties and structure of water, Izd-vo MGU, 1974, 167 p.
[3]. Andreeva N.P., Bunkin A.F., Nurmatov A.A. // Opt. And spectrum. 1999, v. 86, No. 4, p. 579-583.
[4]. Chernin A.D. Cosmic vacuum // UFN, 2001, v. 171, p. 1153-1175.

Quantum-Chemical Study of UV Spectra of Substituted phthalimide-N-oxyl Radicals

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The substituted N-hydroxyphthalimides are studies extensively as catalyst of homogenous oxidation. The active species are phthalimide-N-oxyl radicals (Fig. 1), which can be registered by UV spectroscopy. Because the UV spectra is directly related to the distribution of electronic density within radical, it will be very useful to find appropriate models for UV spectra description.

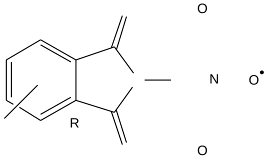

Fig. 1. Structure of PINO

Modeling of UV spectra for radicals was performed by using a B3LYP-DFT method in quantum-chemical Gaussian package with 6-31++G(3df,3dp) basis set. The spectra were described by analyzing the obtained electronic transitions energies and corresponding oscillator strength. Calculated maxima position turns out to be significantly shifted for the PINO itself and its derivatives with a substituent at the 3-position. Results with substituent in the 4-th position are much more consistent with experiment.

System	λmax, nm (experiment)	λmax, nm (calculation)	Maximum oscillator strength
PINO	382	431	0,0035
3-F-PINO	370	435	0,0041
3-Cl-PINO	378	429	0,0038
4-F-PINO	385	380	0,0253
4-Cl-PINO	399	394	0,0218

This result is explained by the difference in intensity of transitions: in case of substituents presence in the 4-th position, oscillator strength is higher by an order of magnitude. Analysis of molecular orbitals (MO) which involved in spectra formation made it possible to distinguish 3 MO groups: group orbitals of NO fragment, as well as group orbitals of the five- and six-membered rings. The lines of UV spectrum for considered molecules are defined by electronic transitions from group orbitals of the six-membered ring to MO of the five-membered ring, and also to NO fragment. Thus, substituent at the 4-position of six-membered ring facilitates electron density transfer from this ring, and substituent in the 3-position greatly hinders it.

Vibrational Spectroscopy of Nanodiamonds-Water Interaction

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The feature of an interaction of water with detonation nanodiamonds (ND) with size of ~5 nmis a resonance of water valence mode ν_{OH} (vibrational band ~ 3000-3800 cm^{-1}) with an overtone 3νD diamond mode (ν_D = 1050-1332 cm^{-1}), as well as a resonanceof the deformation mode of water ν_δ~1640 cm^{-1} and graphite-like shell of ND ν_G=1580-1630 cm^{-1}. The attenuated total reflection (ATR) spectra of wet agglomerates after 7 days and 7 years of their stay in distilled water with subsequent air drying during 8 days have been studied using Fourier spectrometer Termo Scietific Nicolet 6700. It was detected consistent nonmonotonic change of the intensities of vibrational bands of ND D ~ 1300-1330 cm^{-1}, D(k) ~ 1050-1250 cm^{-1} and water ν_{OH}, ν_δ, what is oppositeonesof broadband electronic background.The new anomalies of nanowater in ND have been detected. The intensities of the bands ν_δ,ν_{OH} and ν_{OH}+$\nu_\delta$at first increase and become on 6-14% higher than those in the bulk water, despite the fact that the water in the agglomerates takes only a part of the volume. This phenomenon can be explained by the strengthening of the system of hydrogen bonds (HB) due to the interaction with the surface -OH and -C=O groups of ND, as evidenced by a noticeable increase in the longitudinal-transverse (LO-TO) splitting of the libration mode (620-770 cm^{-1}). It was found out an increase in the ratios of the intensities of the ν_{OH} and ν_δ bands of water from 4.8 to 5.4 with subsequent decrease to 2.8, what characterizes the initial amplification and the subsequent weakening of the HB system. This is confirmed by the offsetof a high-frequency composite component $\nu_{OH1,2}$of water valence band at reducing its content in the agglomerates. A number of difference and total tones in the range of ν_δ and ν_{OH} with acoustic (TA, LA) and optical (TO, LO) collective modes of HB system are observed for the first time. The significant influence of water on the ND vibrational bands D, D(k) is discussed. The regimes of improvement and deterioration of properties of ND, including water induced ND graphitization,amplification and attenuation of bands of C=O and -$CH_{2,3}$ groups. The record abnormal change in the properties of water in the ND agglomerates, including significant amplification of vibrational nonlinearity for residual water, suggests the prospect of their biological and medical applications.

Mutarotation and Light Scattering in the Solutions of Glucose and Fructose

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We proposed a new method for studying the process of generation of inhomogeneities in an aqueous solution by dissolving of glucose. In crystalline form the molecules of glucose are in the form of a ring. In the process of dissolution, the ring opens up and turns into a chain structure then it forms in the ring again. During the achieving of equilibrium, occurs change of the optical activity of glucose solution in water. This occurs because the different forms have different values of optical activity. After equilibration, optical activity of glucose solution becomes constant. This phenomenon is called Mutarotation. Water molecules form aggregates around molecules of glucose whose dimensions are close to the wavelength of light. Also after dissolving glucose in water we can observe light scattering on the aggregates. We have done measurement in distilled and activated water. The easiest way to transfer a water into nonequilibrium state – to heat it. After a while, the water temperature will be the same as the temperature of the surrounding environment. Water returns to equilibrium. We activate water by external electric fields. The most known example – electrolysis of water. In the scheme of two-chamber electrolyzer we get a catholyte, and the other chamber – anolyte.

[1]. Voloshin V.P., Zheligovskaya E.A., Malenkov G.G., Naberuhin Y.I., Tytik D.L., Structures hydrogen bonds grids and dynamics of water molecules in the condensed water systems // Russian Chemical Journal. - 2001. - T. XLV.

Clusters in Clusters: Few Useful Rules Making Binding Energy of the Water Clusters Stronger

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Quantum-chemical calculations of the water clusters structures containing up to 17 water molecules were performed using B3LYP, PBEh1PBE and wB97DX DFT methods of the correlation electron energy accounting and cc-pVTZ basis set. Few levels of the clusters in clusters were observed beginning from dimer to small circle clusters. It was shown that energy of the full cluster decrease when on “dimer” level all dimers have trance configuration. On “circle” subclusters level pentamers and hexamers are preferable due to the angle between monomers in this case most close to tetrahedral one. These rules were tested when $(H_2O)_5$ and $(H_2O)_{17}$ clusters, modeling tetrahedral structures of the ice and low-density water, were analyzed. The structure of the pentamer with T_d symmetry environment of the central molecule is well known. If one considers the four peripheral water molecules like first coordination shell of the central molecule we completed the second coordination shell by additional 12 water molecules. In this cluster 5 water molecules have T_d symmetry environment. We were able to rotate each of four peripheral $(H_2O)_3$groups independently around C_3 axis and have built two configurations presented on Fig.1. The left one contains pentamers and hexamers on “circle” subclusters level, the right one contains trimers and tetramers on “circle” subclusters level. As we expected the first one appears energetically preferable. The IR and Raman spectra of these clusters were analyzed too.

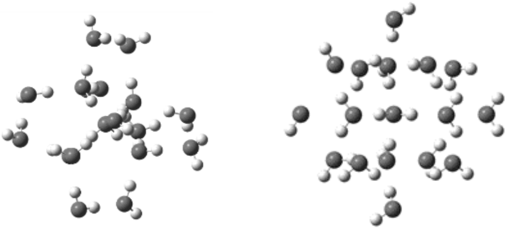

Fig. 1. Calculated structures of the $(H_2O)_{17}$ water cluster

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Interactions of Cation-Anionic Associates of Dyes with Ionic Surfactants

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“Dye+surfactant” and “associate of dyes+surfactant”systems are of great interest in spectroscopy, functional materials and environmental sciences [1]. Our spectrophotometric data demonstrate that ionic surfactants break quinaldine blue (QB^+) associates of phenol red (PR) or bromothymol blue (BT) anions. However, the interaction between the association species and surfactants has a nontrivial specific feature. At hexadecylpyridinium bromide (HDP) concentrations of $4\cdot10^{-5} – 4\cdot10^{-4}$ $mol\cdot l^{-1}$ or dodecylsulfate of sodium (DDS) concentrations of $3\cdot10^{-3} –\ 9\cdot10^{-3}$ $mol\cdot l^{-1}$ the destruction of the association species is kinetically controlled. The absorbance (*A*) of the solution gradually increases with time at invariable dye and of surfactants concentrations (Fig. 1).

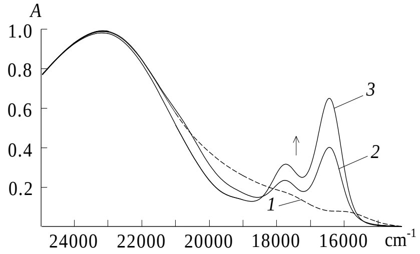

Fig. 1. Evolution of *A* in the DDS-containing “QB^+ +$PR^–$” system. Time *t*, s: *1* – 0, *2* – 180, *3* – 600. Concentrations, $mol\cdot l^{-1}$: QB: $5\cdot10^{-6}$ and PR: $4\cdot10^{-5}$ (*1–3*); DDS: 0 (*1*), $9\cdot10^{-3}$ (*2, 3*).

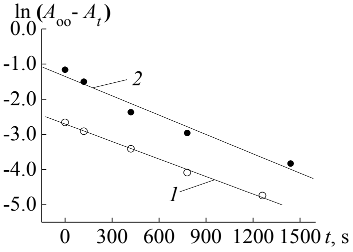

Fig. 2. ln ($A_\infty – A_t$)*vs.* time for the “$QB^+\cdot BT^-$ + HDP” system at $5.0\cdot10^{-6}$ of QB, $2.5\cdot10^{-5}$ of BT, $4.0\cdot10^{-4}$ $mol\cdot l^{-1}$ of HDP; λ: *1* – 560 nm; *2* – 609 nm.

For such first-order reactions, which obey the rate law $\exp(-k\cdot t) = c_t\cdot c_o^{-1}$ the time dependence of a property of the system can be represented as $\exp(-k\cdot t) = (A_t – A_\infty)\cdot(A_o – A_\infty)^{-1}$,$\ln (A_\infty – A_t) = -k\cdot t + \ln (A_\infty – A_o)$ or, in short notation, $Y = B + k\cdot t$ (*k* is the rate constant; $c_t$and c_o are the concentrations of the substance at a time point *t* and at the initial time point ($t = 0$), respectively). As is clear from Fig. 2, the interaction between HDP and the $QB^+\cdot BT^-$ species causes Yto vary linearly with time.

[1].S.A. Shapovalov. The association processes of protolytic forms of dyes in solutions. Self-association : monograph. – Kharkov, 2012. – 218 p. – ISBN 978-966-2445-35-0.

Dimerization of Astraphloxin: Results of Quantum-Chemical Simulation

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Indopolymethines are known for their practical applications in the series of cyanine dyes [1], including the first homologue – astraphloxin (AF; some synonyms: (2Z)-1,3,3-trimethyl-2-[(E)-3-(1,3,3-trimethylindol-1-ium-2-yl)prop-2-enylidene]indole; Astrafloksin, Astraphloxine, Cosmophloxine F). Despite the fact that the aggregated forms of AF are successfully tested in the design of nanosystems [2], its own dimerization has not been studied sufficiently in aqueous solution. This work is devoted to the quantum-chemical simulation of the dimerization of AF^+ cation in a real environment of counterions. We determined the structure and the properties of dimers in different starting variants of spatial tautomers ($2AF^+ + 2Cl^-$ (1), $2AF^+ + 2Cl^-$ (2)) with solvated or unsolvated anions. Conditions of simulation: “MOPAC 2016” [3], RHF approximation, PM7 method, medium is dielectric permeability of water. Some of the results are presented in the table.

Variant of calculation	The wavelength at the maximum of the absorption band, nm			Standard heat of formation, kJ/mol
AF^+	473.9	288.9	202.3	663.6
$AF^+ + Cl^-$	406.6	379.27		642.7
$2AF^+ + 2Cl^-$ (1)	411,8	378.1		92.2
$2AF^+ + 2Cl^-$ (2)	348.6	345.4		182.9
$2AF^+ + Cl^- + 3H_2O$	464.4	404.5		-221.8
$2AF^+ + OH^- + 3H_2O$	464.4	404.5		-310.7

As can be seen, the most energetically advantageous is the dimerization of AF in the electric field of the solvated anion. It is noteworthy that the maxima of the spectral absorption bands of associates for solvated anions of hydroxide and chloride coincide with each other and are located in the visible region.

[1]. S.A. Shapovalov. The association processes of protolytic forms of dyes in solutions. Self-association : monograph. – Kharkov, 2012. – 218 p. – ISBN 978-966-2445-35-0.

[2]. P. Lutsyk et al. Emergence of Additional Visible-Range Photoluminescence Due to Aggregation of Cyanine Dye: Astraphloxin on Carbon Nanotubes Dispersed with Anionic Surfactant // J. Phys. Chem. C. – 2016. – V. 120. – P. 20378–20386.

MOPAC 2016, Version: 17.068L; web-site: HTTP://OpenMOPAC.net.

The Effect of Asymmetry in the Raman Scattering of Liquids

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In the study of molecular substances, mainly, spectroscopic methods of scattering and absorption of light are used. The observed intensity maxima in the spectra of Raman scattering (RS) and infrared absorption (IR) are considered as a manifestation of the frequency of oscillations of interatomic oscillations or chemical bonds. According to the existing representation, the observed oscillation frequencies in the Stokes and anti-Stokes components of the RS spectra should be equal to each other. However, in [1] an asymmetry effect or a difference in the frequency and width of the lines in the Stokes and anti-Stokes components in the Raman scattering in molecular substances was observed (Table 1).

	Stokes shift, cm-1				anti-Stokes shift, cm-1			
Substance	$\nu_{\parallel}$	$\nu_{\perp}$	$\Delta\nu_{\parallel}$	$\Delta\nu_{\perp}$	$\nu_{\parallel}$	$\nu_{\perp}$	$\Delta\nu_{\parallel}$	$\Delta\nu_{\perp}$
$CHCl_3$	260	258	8.3	10.4	265	266	8.8	9.2
	363	364	6.3	10.8	372	370	5.8	9.2
	668	667	6.4	7.3	671	670	5.9	7.3
CCl_4	215	216	11.2	11.2	220	221	9.5	11.3
	311	311	11.0	12.5	319	318	10.8	11.3

In polarization studies, the frequency of the lines in the polarized and depolarized components, which are related to the same intramolecular oscillation, does not coincide.

In this paper we use the notion that all material particles and bodies are formed as a result of vortex processes and condensation of the physical vacuum. According to observational data, the energy density of the surrounding physical vacuum or vacuum liquid is much higher than the energy density of the atomic nucleus [2]. All the real particles, as a result of the condensation of the vacuum liquid, have a natural oscillation frequency with a coherent shell. As a result of field-substance interaction, various harmonics are induced to oscillate frequencies of the particle. They can be considered as induced beats in the frequency of oscillation of a particle or the formation of a vibrating field around a particle. The set of induced beats around the particle has the properties of vibration, so it can be called the wave response function (WRF) [3] of the particle to external influences.

[1]. Erkin Nurmat (Shermatov), Ishburiev R.M., Yakubov A.A. J. Mol. Liquid 1990, vol. 45. p.127-132.
[2]. Chernin A.D. Cosmic vacuum // UFN, 2001, v. 171, p. 1153-1175.
[3]. Erkin N. Shermatov. Superconductivity and human memory. - SPb .: Publishing house of the Polytechnic University, 2006. -172 p.

Peculiarities of the Spectral Properties of Adenine Dimers

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Itis well known that adenine actively absorbs in UV region (λ_{max}= 212 and 260 nm, Fig. 1, curve 3) and exhibit fluorescence at low temperatures (78K [1], λ_{max}= 345) but it is no fluorescent at room temperature. However, we registered the r. t. fluorescence of adenine water solution (λ_{max}=412nm)which appears at $C=4*10^{-6}$ adenine concentration (Fig. 1, curve 1,2). The mechanism of such a fluorescence can be explained due to the adenine-adenine dimmers (AAD) formation[2], [3]. We assume, thatgenerally fluorescence appearance comes from the rigid environment of molecules: if the molecule is trapped in harder environment, which forbid it to loose the energy on heating, so it became fluorescent. Under freezing it takes place for single molecules but at r. t. it may happen because the formation of AAD. Due to the powerful absorption of adenine molecules, they capture energy and then transfer it to the dimmer's energy levels, which are lover that for single molecules Fig.2.

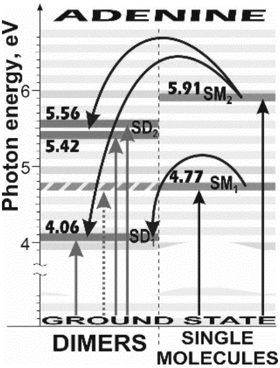

Fig. 1. Adenine absorption(3), fluorescence(2) and excitation of fluorescence(1)

[1] V. Y. Kudrya, V. M. Yashchuk, S. M. Levchenko, V. I. Mel'nik, L. A. Zaika, and D. M. Govorun, 'The Peculiarities of the RNA Luminescence', *Mol. Cryst. Liq. Cryst.*, vol. 497, no. 1, p. 93/[425]-100/[432], 2008.

[2] A. I. Kononov and M. N. Bukina, 'Luminescence excitation spectra reveal low-lying excited states in stacked adenine bases', *J. Biomol. Struct. Dyn.*, vol. 20, no. 3, pp. 465–471, Dec. 2002.

[3] V. L. Rapoport, V. M. Malkin, A. V. Savina, E. A. Safargaleeva, and V. V. Goriuchko, 'Luminescence of stable stacking aggregates of adenine and uracil in water', *Biofizika*, vol. 57, no. 1, pp. 14–20, Feb. 2012.

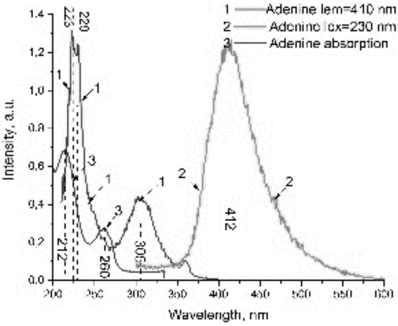

Fig. 2. Energy levels

Water in Ar Matrices: Confinement with Changing Sizes

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Research is devoted to the investigation of the changing of the cluster structure of water confined in Ar matrices with changing temperature. Usually one uses the porous materials for the investigation of the peculiarities of the structures of confined water [1]. However, it gives no possibility to study the structure of confined water at the changes of the volume of the cavities. The temperature evolution of the volumes of cavities in cryo-matrices allows investigating evolution of cluster structure of water from gas phase to confined condensed phase [2].

The research was supported by the State Fund for Fundamental Research of Ukraine in the frame of bilateral Ukrainian-Belarusian agreement (grant F73/31 – 2017).

[1]. Francesco Mallamace, Matteo Broccio, Carmelo Corsaro, Antonio Faraone, Domenico Majolino,Valentina Venuti, Li Liu, Chung-Yuan Mou, and SowHsin Chen, //Evidence of the existence of the low-density liquid phase in supercooled, confined water//PNAS, January 9, 2007, vol. 104, no. 2, pp. 424–428.

[2]. V. Pogorelov, I. Doroshenko. Low Temp. Phys. 2016, V. 42, № 12, p. 1487–1491.

Molecular Isomerization of 1-butanol in Argon Matrix Isolation: FTIR Study and High-Level *ab initio* Calculations

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Rotational isomerism is well-known effect, which has been studied for different types of chain molecules with every possible experimental and theoretical techniques. Nevertheless, alcohol molecules are generally neglected when it comes to conformational analysis. Ethanol, 1-propanol and 1-butanol have been studied a lot for isomerization in gaseous phase.

Another important part of alcohols investigation is devoted to clusterization of molecules in condensed phase and in matrix isolation. Such researches are often provided comparing experimental and computed spectra of different clusters. The erroneous of such approach is comparison of wide experimental bands with narrow theoretical ones. As a result, correctness of such comparison cannot be estimated.

The aim of this work is investigation of 1-butanol molecular isomerization in Ar matrix isolation, its influence on clusterization process and on the width of vibrational bands in FTIR spectra. For such approach, FTIR spectra of 1-butanol in cryo matrix were registered with 1 cm^{-1} resolution. Molecular isomers of alcohol were calculated using high-level *ab initio* methods for optimization (ROCBS-QB3) and anharmonic spectra calculations (MP2/6-311G(2d,d,p)). Alcohol clusters containing different isomers (Fig. 1) were studied with the same level of theory.

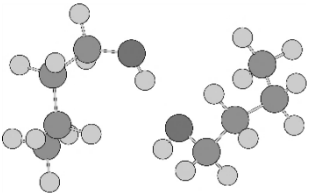

Fig. 1. 1-butanol dimer structure with GG't-G'G'g molecular isomers inside

Acknowledgment

The work was carried out in the frame of Ukrainian-Lithuanian bilateral agreement supported by Ministry of Education and Science of Ukraine. FTIR spectra of 1-butanol in matrix isolation were registered in the Laboratory of Fourier-transform infrared absorption spectroscopy at the Vilnius University, Lithuania. The authors thank Prof. V. Balevicius and Prof. V. Sablinskas for the opportunity to perform such experiments.

Effect of Irradiation on the IR Spectra of Solutions of Anticancer Drugs

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The work purpose – analysis of the effect of high-energy electron irradiation of solvent (distilled water or saline) on the activity of the dissolved anticancer drugs to increase their therapeutic activity. The measurements used drugs doxorubicin (doxorubicin, "Pharmacia Italia SpA", Italy) and Conium (Weleda, Germany). The solvent used was a solution of sodium chloride in concentration 9 mg/ml, produced by LLC "Novofarm - Biosynthesis", Ukraine. Measured dependence of the absorption (A) of solutions drugs of the energy of a photon (ε) in the infrared range of light The value of the absorbed dose of irradiation (I) was 5 (I_1), 10 (I_2), 25(I_3), 40(I_4) and 80(I_5) kGr. Electrons energy was 2.0 MeV. The measurements were carried out on IR - Fourier spectrometer Bruker IFS 66. We have identified the coefficients of Pearson's correlation between spectra A(ε, I=0) and A(ε, Ii) i=1..5. It was shown that preliminary irradiation of the solvent does not change significantly medical drugs (in all cases the correlation coefficient exceeds the critical value). Irradiation change only some parts of the spectra in the vibrational range. This is due to the irradiation influence of the solvent on the conformational state of the molecules of drugs.

Emission Centres in Solid Solutions with Silver and Copper Impurity

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In our studies, the energy structure of absorptive and radiative centres in solutions of inorganic salts and acids which contained the silver (copper) ions as an activator is investigated. Absorption, luminescence and photoexcitation spectra of the solutions with silver (copper) ions (10^{-3} – 10^{-1} mol/l) are explored in the temperature range of 4.2–290 K.

The spectral distribution of the emission from the solutions activated with silver (copper) ions does not depend on the concentrations of silver (copper) ions and anions of the solvents, as well as on the state of freezing of the solution.

Such solutions are characterized by three types of structured bands of absorption (excitation) and emission.

The observed bands may be associated with the certain transitions in a free Ag^+ (Cu^+) ion, the energy levels of which are deformed due to an interaction with external environment.

The study of silver (copper) impurity in examined solid solutions allowed us to elucidate the energy structure of absorption and emission centers for such systems.

The analysis of spectral characteristics of silver (copper) ions in solutions of inorganic compounds allows us to develop the high-sensitivity luminescent techniques of testing the silver (copper) microimpurity in those solutions.

Analyzing the spectral characteristics of silver (copper) ions in the inorganic solutions confirms the validity of an ionic model of absorption and emission centers for comlexes in investigated solutions.

3

Crystals

Luminescence Mechanisms in $ZnMoO_4$ Scintillation Crystals

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The scintillation properties of zinc molybdate crystals $ZnMoO_4$ are intensively studied at present since these crystals are considered as perspective scintillation materials for various experiments in particle physics. The luminescence spectra of undoped $ZnMoO_4$ crystals usually reveal two components peaking near 530 and 620 nm. According to current opinion, the short wavelength component originates from radiation annihilation of self-trapped excitons localized on MoO_4 groups of the crystal. However, the origin of the long-wavelength component is still the subject of discussion. According to assumption made by several authors, this component should be related to existence of the oxygen vacancies in the crystal lattice. As result, the oxygen-deficient molybdate groups, MoO_3, are formed. The present work is aimed to examine this assumption in complex experimental and computational studies. Dependences of the long-wavelength emission component intensity and other luminescence characteristics of the zinc molybdate on concentration of the oxygen vacancies are analyzed for the set of samples synthesized at different conditions.

The polycrystalline samples of the $ZnMoO_4$ with various concentration of the structural defects were synthesized by solid-state reaction method. The luminescence properties were studied in the VUV region of excitation photon energies on SUPERLUMI station at HASYLAB (Hamburg, Germany). Additional bands in the optical absorption spectra were characterized by diffuse reflectance spectroscopy. The influence of several kinds of defects (V_o, V_o+V_{Zn} and W_{Mo}) on the electronic structure of $ZnMoO_4$ crystal was studied by FP-LAPW calculation method [1].

Obtained results and their analysis support assumption on the defect-related origin of the long wavelength emission component of zinc molybdate.

[1]. P. Blaha, et al, 2001. ISBN 3-9501031-1-2.

Terahertz Study of the Lattice Dynamics of the Rare-Earth Binary Molybdates M*Re*$(MoO_4)_2$

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We report a systematic study of low-energy lattice vibrations in the binary molybdates M*Re*$(MoO_4)_2$ (M^+ is an alkali metal ion and Re^{3+} is rare-earth ion). A layered crystal structure and low symmetry of the local environment of the Re^{3+} ion cause the appearance of vibrational and electronic excitations in Terahertz frequencies. The interaction between these excitations leads to sophisticated dynamical properties, including magnetic field induced phase transitions and non-linear effects in paramagnetic resonance spectra [1,2]. The THz study in magnetic field allows for the clear distinction between lattice vibrations and electronic excitations.

We have measured the THz transmission spectra of M*Re*$(MoO_4)_2$ with different composition (M = K, Rb, Cs, and *Re* = Tm, Er, Dy, Gd, and Y). Based on the obtained results, we developed the quasi-one-dimensional model which describes the lattice vibration on the microscopic level, and results of our calculations agree with previous Raman and ultrasound studies. An excellent agreement with the experimental results reveals that the low energy lattice vibrations in binary molybdates can be well described within the relatively simple quasi-one-dimensional model. This finding is very important for the interpretation of the abovementioned non-linear effects in these compounds because it allows for the exact calculation of the lattice distortion induced by high power THz radiation. It is important to note that the suggested model is rather general and applicable for other layered systems.

[1]. M. J. M. Leask, O.S. Tropper, M.L. Wells. Antiferrodistortive Jahn-Teller ordering in $KDy(MoO_4)_2$ // J. Phys. C: Solid State Phys. – 1981. – V. 14. – p. 3481 - 3498.

[2]. D. Kamenskyi, S. Poperezhai, P. Gogoi, H. Engelkamp, J. C. Maan, J. Wosnitza, and V. Kut'ko. Interaction of electronic excitations of Tm^{3+} ions with acoustic vibrations in $KTm(MoO_4)_2$// Phys. Rev. B – 2014. – V. 89. – p. 014410

Spectral Analysis of Diamond Deformations: Amplification of Vibrational Bands and Initiation of Inhomogeneues of Monocrystals

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We have established that the formally linear Young's modulus **E** and the shift **G** are related to the resonance nonlinear-wave interactions of vibrational modes and vibrational-electron interaction. The last lead to changes in the electronic states (ES) and chemical bonds. For spectral studies of deformations of solids, single crystals of diamond are ideally suited. This is due to the wide area of their transparency, the presence in the Raman spectra (RS) of the sharp and intense D line of 1332 cm^{-1} and the traditional use of diamond anvils (AN) in the high-pressure region P ~ 20-100 Gpa. RS diamonds were studied using a TRIAX 552 spectrometer, Jobin Yvon with a CCD detector (514.5 nm excitation ~ 1-5 mW, focusing 2 μm). At $P \neq 0$, narrow D lines transform into wide DP bands, the sharp high-frequency (HF) edge of which shifts at a speed of 2.4 cm^{-1}/GPa and often exceeds 1400 cm^{-1}. An increase with increasing P of the changes in the electronic polarizabilities is established for oscillations $d\alpha$ / dq, which determine the intensity of the maxima of the observed bands. It is shown that the RF maxima of the DP bands in the case of elastic deformation near the working surface of the AN (0.3-0.6 mm, face (001)) at P~10 GPa are amplified ~ 15 times, and with increasing P up to 25-30 GPa decrease 3-5 times, which characterizes the manifestation of inelastic deformation. The integrated intensities of the D_P bands increased in 30-80 times, which indicates an abnormal change in the ES of strongly deformed AN. The amplification of nonlinear wave processes for deformed AN ~5 times, which determine the vibrational relaxation rates, is proved. For the first time, a discrete structure of the D_P bands was observed, containing more than 4 marked maxima, which is associated with the appearance of spatial inhomogeneity in the height of the AN. This structure of D_P bands was significantly enhanced by a shear deformation of 180°-200°. At the same time, the recorded pressure increased ~ 1.5 times. The obtained results indicate the prospect of the further development of the nonlinear quantum concept of strength and plasticity and the raising of the classical phenomenological theory of elasticity and deformation of solids to the level of fundamental science.

$Tl_{10}Hg_3Cl_{16}$ Crystals and Determination of Their Electronic Structure

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Ternary thallium halides with a common formulae Tl_4HgX_6 (X=Br, I) are of increased interest as very prospective materials for application in ionizing radiation detectors, temperature sensors and non-linear optical devices [1]. No analogous chlorine-containing compound belonging to the Tl_4HgX_6 system has been found to exist. Nevertheless, the formation of a phase at a similar composition that is described by the formula $Tl_{10}Hg_3Cl_{16}$ has been reported [2]. Fig. 1 presents the survey X-ray photoelectron (XP) spectra of the $Tl_{10}Hg_3Cl_{16}$ single crystal that were measured for both pristine and Ar^+ ion-bombarded surfaces.

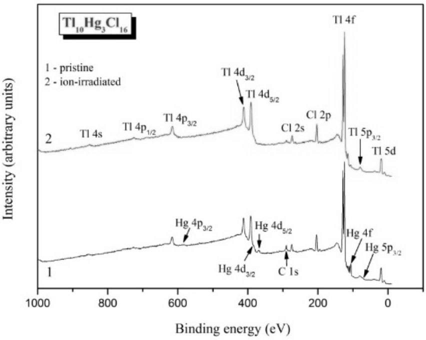

Fig. 1. Survey XP spectra recorded for (1) pristine and (2) Ar^+ ion-bombarded surfaces of the $Tl_{10}Hg_3Cl_{16}$ crystal.

From Fig. 1, it is apparent that all the fine-structure features of the survey XP spectra, except of the C 1s core level of carbon-containing adsorbates, are attributed to the core-levels of atoms constituting $Tl_{10}Hg_3Cl_{16}$. Extremely low hygroscopicity is a characteristic of the $Tl_{10}Hg_3Cl_{16}$ single crystal surface. This property is rather important when handling the $Tl_{10}Hg_3Cl_{16}$ compound in optoelectronic or nano-electronic devices operating at ambient conditions.

[1]. D. Kahler, et al. Nucl. Instrum. Methods Phys. Res. A 652 (2011) 183–185.
[2]. J. Huart, Bull. Soc. Fr. Miner. Cristal. 89 (1966) 23–25.

The Features of Conductivity of $TlInS_2$ Ferroelectric C- and 2C-Polytypes

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An important feature of semiconductors-ferroelectrics β-$TlInS_2$ is the existence of phase transitions (PT) with the creation of phases with modulated structures both commensurate (CP) and incommensurate (IP). To clarify the mechanisms of PTs the information about the electrical conductivity for crystals $TlInS_2$ of different polytypes in temperature ranges of the existence of IP (214 K–194 K) and CP (T<194 K) is required. Therefore, in presented work it was experimentally investigated the temperature dependence of electrical conductivity $\sigma_\perp$(T) on DC for C- and 2C-polytypes of $TlInS_2$ crystals during the cooling in temperature range 100 K–300 K as initial samples, and after X-rays irradiation the samples with doses of 0,9 kGy and 2,9 kGy. It was revealed that temperature dependences for such polytypes demonstrated significant differences. The increasing of the conductivity during the cooling in the temperature interval of the IP existence was observed for C-polytype, meanwhile for 2C-polytype the conductivity monotonically decreased in the whole temperature range (Fig. 1).

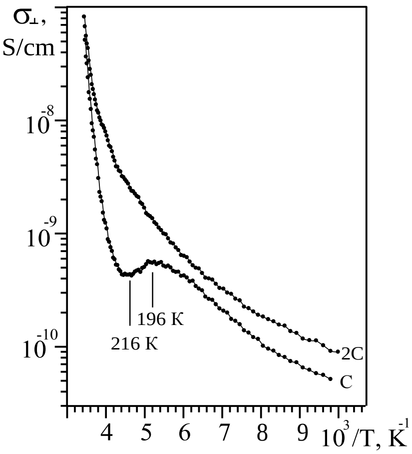

Fig. 1. The temperature dependence of the $TlInS_2$conductivity

It was shown that in temperature range 160 K–120 K for C- and 2C-polytype observed the hopping conductivity with a variable jump length, caused by the existence of localized states near the Fermi level. It was revealed that X-ray irradiation of C-polytype samples leads to smoothing the anomalies on the dependence $\sigma_\perp$(T) in temperature range of IP (214 K–194 K). The mechanism of the conductivity increasing at the temperatures 214 K–194 K was suggested based on tunneling the charge carriers through the system of potential wells, which are created in field of incommensurate potential of the superlattice. The influence of defects on the formation of such potential under irradiation was also discussed.

The Spectra of X-ray Luminescence and Photoluminescence of ZnSe Single Crystals

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The experimentally investigated spectra of X-ray luminescence (XRL) and photoluminescence (PL) ZnSe from 400 to 1200 nm at different temperatures (8, 85, 295 and 430 K) and 3 excitation intensity levels. The XRL and PL spectra of high-resistance ZnSe samples consist of two main luminescence bands with maxima at 630 nm (1.92 eV) and 970 nm (1.28 eV). The band with a maximum in the case of 630 nm is caused by the complex center including vacancy of zinc, and a band with a maximum at 970 nm is caused by the complex center with vacancy of selenium or an impurity of copper.

In case of change of the intensity of X-ray and photo excitation, the spectral positions of the maxima and form of the bands do not change. A comparison of the XRL and PL spectra shows that they are similar to one another. This means that the observed bands are recombination for x-ray and band-to -band photoexcitationat these temperatures, which is confirmed by the presence of these bands in the spectral composition of phosphorescence and thermally stimulated luminescence.

At the high temperatures (420 K), due to the effect of thermal extinction of the luminescence, the intensity of the XRL is falling so heavily that it becomes impossible to register the spectrum. PL spectrum was able to register at 420 K and found that at this temperature there is only one greatly extended the short wavelength band.

The luminescence temperature quenching of both luminescence bands is observedat T > 100 K. However, the temperature dependences of the bands are different, which causes absence of 970 nm band at 420 K. It should be noted that at low temperatures even in the case of increase in the sensitivity of the recording system by two orders are not observed in either edge luminescence or luminescence of donor-acceptor pairs.

Recently, an interesting feature of ZnSe crystals has been discovered, that on recombination center, which produces luminescence with a maximum at 1.92 eV, the two opposite mechanis

Influence of the H-Bonding to IR Spectra of Triphenyl Phosphite

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IR spectra of triphenyl phosphite (TPP) were measured in the liquid, glassy and glacial phases and in the stable and metastable crystalline phases.The differences between the IR spectra measured in different phases which are observed in the 3020-3080 cm^{-1} spectral region can not be explained by the presence of different conformers. The aim of our work is to explain the observed differences in the IR spectra.

The conformers differ from each other by the angles of rotation of the benzene rings, which are twisted with respect to C-O bond.

Experimental and simulated IR spectra were analyzed. The structure and geometrical parameters of the conformers most close to the structure of hexagonal and monoclinic polymorphs of TPP according to X-ray diffraction data were determined.

The study of the IR spectra makes it possible to establish the presence of a weak intermolecular H-bonding between the oxygen atom and hydrogen atom of a phenyl ring (C-H···O). The experimental IR spectra were interpreted. It was shown, that the IR spectra of the glass, glacial and liquid phases are superposition of the calculated IR spectra of conformers and dimers with weak hydrogen bond (Fig. 1).

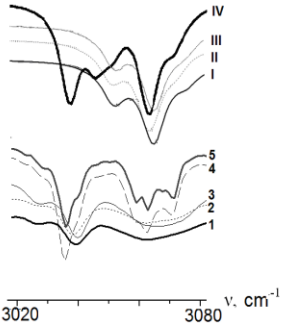

Fig. 1. Experimental (1 – liquid, 2 – glass, 3 – glacial, 4 – stable phase, 5 – metastable phase) and calculated IR spectra of the conformers (I–III) and dimer (IV).

Synchrotron-Radiation Induced Renormalization of Luminescence Spectra from Atomic Cryocrystals

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Because of strong interaction with phonons the excitons and holes in atomic cryocrystals (AC – solid Xe, Kr, Ar, and Ne) are self-trapped, and a wide range of electronic excitations are created in samples: free excitons (FE), atomic-like (A-STE) and molecular-like self-trapped excitons (M-STE), molecular-like self-trapped holes (STH) and electrons trapped at lattice imperfections. Radiative decay of these excitations forms the wide range of luminescence bands in the luminescence spectra from AC [1]. The processes of formation of A-STE and M-STE centers are accompanied by a considerable energy release to the crystal lattice which exceeds the binding energy of atoms in AC. The STE-luminescence is a sensitive tool for investigation of a local surrounding of the STE-center [2]. It was used as a short-range probe in studies of defect formation induced by electronic transitions and creation of charged centers in atomic cryocrystals. The analysis of the STE-luminescence spectra under different excitation conditions, excitation energies and crystal-growth conditions made it possible to investigate the kinetic parameters of renormalization of the set of electronic excitations in atomic cryocrystals.

The photoluminescence experiments were carried out at the SUPERLUMI experimental station at HASYLAB, DESY, Hamburg. Selective photon excitation was performed with $\Delta\lambda=0.2$ nm. The luminescence was spectrally dispersed with 0.5 m Pouey monochromator with $\Delta\lambda=2$ nm. In luminescence spectra of AC the *M*-band is formed by radiative decay of molecular self-trapped excitons (M-STE) [3]. The interplay of various subbands of *M*-band as a result of selective photon excitation of AC-sample in the energy range $E_1<E<E_g$ (E_1 is the threshold energy for the defect subband excitation, E_g – the gap energy) allows to reveal the internal structure of various luminescence subbands and to recover the general scheme of branched relaxation pathways in which these subbands are formed.

[1]. A.N. Ogurtsov. Cryocrystals Modification by Electronic Excitations. – Kharkiv: NTU "KhPI", 2009. – 368 p.
[2]. A.N. Ogurtsov, O.N. Bliznjuk, N.F. Kleshchev, N.Yu. Masalitina // ITE. – 2013. – N. 4. – P. 24 – 31.
[3]. A.N. Ogurtsov, N.Yu. Masalitina, O.N. Bliznjuk. In: Contributed Papers of the 6th Conference on Elementary Processes in Atomic Systems. – Bratislava: Comenius University, 2014. – P. 242 – 244.

Luminescence Properties of Pr^{3+}-doped Bi-containing Phosphates and Molybdates

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The great diversity of oxide materials doped with Pr^{3+} ions have been actively studied as red emitting phosphors for application in light-emitting diodes, plasma display panels, field emission displays etc [1]. It is known the Bi-containing compounds are good hosts for rare-earth (RE) ions because of similarity of ionic radii and electronic affinity of Bi^{3+} and the RE^{3+} ions. Wide absorption bands in ultraviolet-violet spectral regions and high probability of energy transfer from host to RE ions are other reasons which make Pr^{3+}-doped Bi-containing phosphates and molybdates attractive luminescent materials for abovementioned applications.

Three series of solid solutions with compositions $Bi_{1-x}Pr_xPO_4$, $KBi_{1-x}Pr_x(MoO_4)_2$ and $K_2Bi_{1-x}Pr_x(PO_4)(MoO_4)$ (x = 0.01 - 0.10) have been prepared by solid state reactions. As starting materials Bi_2O_3 (99.99%), $(NH_4)_2HPO_4$ (99.999%), K_2MoO_4 (99.99%),MoO_3 (99.99%) in stoichiometric ratioshave been used without additional purification. compounds fromof and Pr_6O_{11} (99.999%). The annealing temperature for each sample has been increasing from 550 ºC to 700 ºC for $KBi_{1-x}Pr_x(MoO_4)_2$, 780 ºC $Bi_{1-x}Pr_xPO_4$and 800 ºC for $K_2Bi_{1-x}Pr_x(PO_4)(MoO_4)$. The powders were re-grinded after each temperature treatment up to the samples' color change from grey to greenish at the final stage of annealing. The phase composition of prepared samples was determined by X-ray diffraction and IR spectroscopy methods.Photoluminescence properties were studied with using of diode-pumped laser (λ_{ex} = 473 nm) and powerful xenon lamp DXeL1000 (1000 W, working range 200 – 650 nm) excitation sources.

It was found that the studied samples reveal intensive red luminescence when excited in the range of the ${}^3H_4 \rightarrow {}^3P_J$f-f transitions in the Pr^{3+} ions. The most intensive peaks in photoluminescence spectra are related with ${}^3P_0 \rightarrow {}^3H_6$ (602.8 nm) and ${}^3P_1,{}^1I_6 \rightarrow {}^3F_2$ (610 – 635 nm) transitions in the Pr^{3+} ions.Redistribution of PL bands intensity is clearly observed with increasing of praseodymium content.

[1]. C.C Lin, A. Meijerink, R.-S. Liu. Critical Red Components for Next-Generation White LEDs // J. Phys. Chem. Lett. – 2016, – V. 7. – № 3. – p. 495–503.

Vibrational Properties of Zinc Peroxide

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Nanocrystalline ZnO_2 powders were directly produced by hydrothermal process using zinc acetate as precursor and hydrogen peroxide as oxidant agent. Vibrational properties were characterized using Bruker VERTEX 80v FTIR spectrometer and Renishaw Micro Raman spectrometer.

Calculations of fundamental vibrations of the ZnO_g have been performed by using hybrid exchange density functional theory to determine equilibrium geometries and phonon frequencies. The CRYSTAL14 computer code was used.

Calculated end experimental fundamental vibrations of ZnO_2 were discussed.

FTIR and DSC Studies of Binary Mixtures of Long-Chain Aliphatic Compounds

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In this work, we studied and compared the physicochemical properties of the binary mixtures of biochemically important long-chain aliphatic compounds formed of saturated fatty acids with alkyl chains containing even carbon atoms of 12, 18 or 22 - lauric (kC12), stearic (kC18) or behenic (kC22) acids, and (2) cationic cetyltrimethyl-ammonium bromide (CTAB) and anionic fatty acids - kC12, kC18 or kC22 surfactants. Fatty acids are anionic surfactants under their deprotonated forms. They are surfactants with both biodegrability and low toxicity. Fatty acid molecules can self-assemble under various shapes in an aqueous solution. These self-assembled structures can vary under such stimuli as pH, and temperature due to changes occurring at the molecular level. These specificities make them surfactants of special interest to tune the properties at a macroscopic scale. The binary mixtures of the surfactants have been analyzed at different mixed ratios ($0.2 \leq x \leq 0.8$) by means of differential scanning calorimetry (DSC) and Fourier transformed infrared spectroscopy (FT-IR). A Perkin-Elmer Model 8000 was used for DSC measurements in the temperature interval of 20-150°C with the heating and cooling rate of 8°/min. FT-IR measurements were carried out using a Bruker IFS-88 model (4000-380 cm^{-1}, 2 cm^{-1} resolution). For the first time, rich phase behaviors have been observed for the binary mixtures upon heating with a series of phase transitions. The possible molecular mechanisms of successive solid state phase transitions are discussed with regard to the molecular interaction and hydrocarbon chain conformational changes in the mixtures. The revealed complicated character of the phase diagrams for these systems may have an important effect on the development of industrial separation and purification processes for fatty acids, as well as on the creation of new products based on these compounds for biology, medicine, and pharmacology.

Optical Properties of Thin Erbium Oxide Films Formed by Rapid Thermal Annealing on Substrates with Different Structures

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Rare earth oxides (REOs) are often considered as an alternative to SiO_2 films used in silicon oxide/silicon carbide structures. High transparency in the visible spectral range, chemical and thermal stability makes REOs promising for antireflective coating in photoelectric devices and for the replacement of silicon oxide in field-effect transistors. An interface with low recombination losses is an important requirement for optical coatings in semiconductor devices. The structural defects penetrating during high temperature process into film grown on semiconductor substrate can significantly degrade the device characteristics. Porous interlayer between substrate and epitaxial layer can reduce this effect.

This report deals with the comparative analysis of optical properties of thin erbium oxide films formed by rapid thermal annealing (RTA) on crystalline silicon carbide and the substrates with porous silicon carbide used as a buffer layer between Er_2O_3 film and crystalline silicon carbide.

Analysis of the distribution profiles of elements in SiC/por-SiC/ErO_x and SiC / ErO_x structures obtained by Auger electron spectroscopy has revealed that with an increase of RTA time the oxide film composition in both cases approaches the stoichiometric parameters: $N_O/N_{Er} \approx 1.25–1.6$ for SiC/por-SiC/ErO_x structures and $N_O/N_{Er} \approx 1.6–1.7$ for SiC/ErO_x structures. The thickness of oxide layer is 80-100 nm in structures with a por-SiC buffer layer and 100–150 nm in structures without porous layer. In SiC/por-SiC/Er_2O_3 structures more blurred boundary between the erbium oxide film and por-SiC buffer layer is observed. The increase of RTA time leads to increase of transmission in spectral range of 400-800 nm both in 6H-SiC/Er_2O_3 and SiC/por-SiC/Er_2O_3 structures. The increase of transmittance for the oxidized erbium films is caused by increase of the fraction of Er oxide film with stoichiometric composition in comparison to the sub-oxidized metal layer.

RTA method allows to form thin layers of stoichiometric erbium oxide on por-SiC surface.

Anomalous Behavior of the Thermal Conductivity of Unsubstituted and Bromo-Substituted Benzophenones

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Derivatives of benzophenone are very interesting molecular substances. These compounds form molecular crystals and they have low-energy intramolecular modes which exist along with phonons that are either strongly associated with acoustic phonons or stands slightly above the phonon spectrum. The interaction between phonons and the intramolecular modes leads to various anomalies in optical and thermal properties.

The results of measurements of the thermal conductivity of a single-crystal unsubstituted benzophenone in thermodinamic stable phase in the temperature range 4.7 - 270 K are presented. The obtained results were compared with the data for two polymorphs of 4-bromo-substituted benzophenones [1-2]. It was shown that the thermal conductivity of unsubstituted and bromo-substituted benzophenones in wide temperature range can be represented as the sum of two terms $k = k_1 + k_{TA}$, where the first term κ_1 corresponds the thermal conductivity of full orientational-ordered crystal and the second term k_{TA} corresponds for activation process. It was suggested thermal activation process arises from the thermally stimulated excitation jumps caused intramolecular vibrations between benzophenone molecules in the crystal.

[1] M.A. Strzhemechny, A.I. Krivchikov, A. Jeџowski, D.I. Zloba, L.M. Buravtseva, O. Churiukova, and Yu.V. Horbatenko, New thermal conductivity mechanism in triclinic 4-bromobenzophenone crystal // Chem. Phys. Lett. – 2016, 647, 55.
[2] O.O. Romantsova, Yu. V. Horbatenko, A.I. Krivchikov, O.A. Korolyuk, G.A. Vdovichenko, D.I. Zloba, O.S. Pyshkin, Anomalous heat transfer in two polymorphs of para-bromobenzophenone // Low Temperature Physics, - 2017, 43, 3, 395-399.

Terahertz Spectroscopy of the Jahn-Teller Phase Transition in $KDy(MoO_4)_2$

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$KDy(MoO_4)_2$ belongs to the family of double alkali rare-earth molybdates. Atlow temperatures, this compound exhibit various fascinating effects due to the interaction of the electronic and lattice subsystems. In $KDy(MoO_4)_2$, the structural phase transition (PT) induced by the cooperative Jahn-Teller effect goes in two steps via the intermediate phase ($T_{C1}\approx 14.5$ K and $T_{C2}\approx 11.5$ K) [1,2]. Additionally, at 4.2 K the magnetic field applied in a certain direction (along the maximal value of the g-factor) leads to the structural transformation of the crystal [3].

In this work, we present the results of terahertz study of low-energy excitations of Dy^{3+} ions in $KDy(MoO_4)_2$ in the range of temperatures in the vicinity of PT. FIR transmission spectra of $KDy(MoO_4)_2$ were measured between 10 and 120 cm^{-1} (0.3 ÷ 3.5 THz) in temperature interval 1.4 – 24 K and in magnetic fields up to 15 T. The THz transmission spectra exhibit a clear modification when the system goes over the phase transition. The first excited Kramers doublet of the ion Dy^{3+}, which lies 18 cm^{-1} above the ground state shifts upon the cooling below the phase transition to 27 cm^{-1}. We found a few additional features in the spectra taken at temperatures below PT. The main findings are an additional electron mode at about 22 cm^{-1} and changes in the intensities of the electron modes depending on the light polarization. On the presentation, we are going to discuss the possible mechanisms of formation observed THz spectra and microscopic mechanism of the PT.

[1]. I. Zvyagin, T. S. Stetsenko, V. G. Yurko, and R. A. Vaishnoras. Low-temperature Phase Transition in $KDy(MoO_4)_2$ Produced by the Cooperative Jahn-Teller Effect // JETP Lett. – 1973. – V. 17. – N. 4. – p. 135 - 137.
[2]. Yu. N. Kharchenko. Breakdown of the antiferrodistortion Jahn-Teller ordering in a $KDy(MoO_4)_2$ crystal in magnetic field: the intermediate phase formation // Low Temp. Phys. – 1996. – V. 22. – N. 4. – p. 306 - 310.
[3]. M. J. M. Leask, O.S. Tropper, M.L. Wells. Antiferrodistortive Jahn-Teller ordering in $KDy(MoO_4)_2$ // J. Phys. C: Solid State Phys. – 1981. – V. 14. – p. 3481 - 3498.

Electronic Structure and Peculiar Properties of RCoO$_3$ Compounds

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Among the transition metal perovskites, the cobalt-based ones exhibit the richest variety of valence and spin states. These compounds have unusual magnetic, electronic, and structural properties, which remain the subject of controversial discussion.

Whereas the magnetic susceptibility of YCoO$_3$ appeared to be rather small, the magnetic susceptibilities of LaCoO$_3$ and EuCoO$_3$ compounds demonstrate pronounced and different temperature dependencies (Fig. 1). In LaCoO$_3$ the magnetic susceptibility χ shows a maximum around 100 K that is ascribed to a spin-state transition from a non-magnetic insulating state at low temperatures to a magnetic insulating state at higher temperatures. At higher temperatures, a metal-insulator transition occurs, which is accompanied by an increase of the magnetic moment. Also, the pressure effect on magnetic susceptibility was studied experimentally, and found to be remarkably different for these compounds.

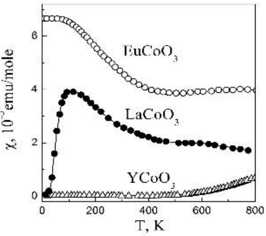

Fig. 1. Temperature dependencies of the magnetic susceptibility of *R*CoO$_3$.

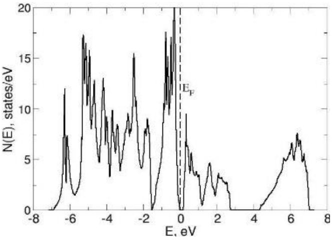

Fig. 2. Density of electronic states $N(E)$ of LaCoO$_3$

In order to shed light on these experimental data, we have investigated the electronic structure and magnetic properties of YCoO$_3$, LaCoO$_3$ and EuCoO$_3$ compounds with DFT-based methods. We have used the full potential linear augmented plane wave (FP-LAPW) method and the pseudopotential Quantum Espresso implementation with the GGA and LDA approximations for exchange-correlation effects. Also, we had to employ LDA+U approach to describe strong correlations and appearance of a small energy gap. The calculated density of electronic states $N(E)$ of LaCoO$_3$ is presented in Fig. 2. The calculations have revealed two local minima of total energy, for non-magnetic and a magnetic state. The energy difference between these states is very sensitive to the lattice distortions.

Crystal Structure, IR and Raman Spectra and DFT Modeling Studies of Two Salts of 2-Chloro-4-nitroaniline with HBr and H_2SO_4

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New crystals were obtained in reaction of 2-Chloro-4-nitroaniline (2Cl4NA) with respective acid in methanol solution. The 2Cl4NA-H^+•$[HSO_4]^-$ (**1**) crystallizes at room temperature in monoclinic crystal system, space group is $P2_1/c$, with lattice parameters: a=16.1771(6), b=4.95335(16), c=12.8431(5) Å, β=101.584(4)°, V=1008.17 $Å^3$ and Z=4. The 2Cl4NA-H^+•Br^- (**2**) crystallizes in orthorhombic $P2_12_12_1$ space group, with lattice parameters: a=5.72152(9), b=7.90017(17), c=20.2729(4) Å, V=916.355 $Å^3$, Z=4. The asymmetric unit for both compounds consists of one cation and one anion. The structure is stabilized by N−H···O and O−H···O hydrogen bonds for **1**, and N−H···Br hydrogen bonds for **2**. In the crystal structure of **1** cations and anions compose layer of hydrogen bonds parallel to *bc* plane. In the case of **2** hydrogen bonds form a ladder-like chain pattern propagated along *a* crystallographic direction.

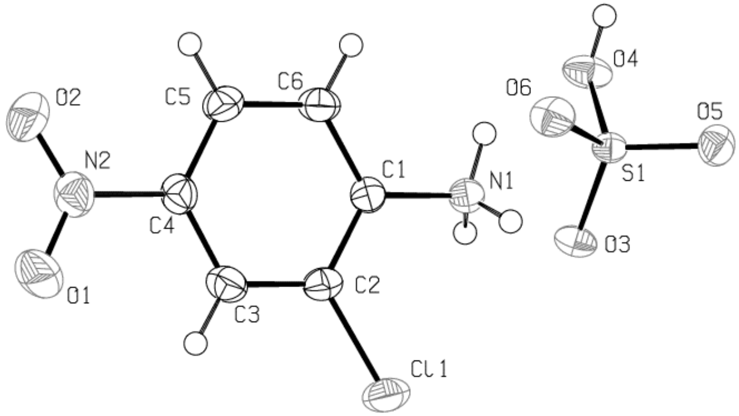

Fig. 1. Molecular structure of **1** according to X-ray diffraction data.

The experimental IR and Raman spectra were interpreted basing on DFT calculations. The theoretical and observed frequencies have been compared and several stretching and deformation modes confirm the presence of intermolecular hydrogen bonding in the title crystals.

Luminescence of Polycrystalline Scintillators Based on Stilbene

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Luminescence of organic crystal can be used to detect fast neutrons and ionizing α- and β-radiation which are most harmful for the human body. One of the ways to improve efficiency of the short radiation detection is to increase the area of the sensing element of the recording setup. New types of detectors with large areas can be prepared on the base of composite materials and by sintering (cold and hot pressing).

In this paper, we have studied the luminescence (PL) spectra of single crystals and pressed polycrystals of trans-stilbene within wide temperature range (5-300 K). Since high-quality scintillators must be cleaned of impurities and defects, stilbene single crystals were prepared by different methods: by sublimation, from dichloroethane solution and by directional crystallization. It is shown that stilbene single crystal film after sublimation shows very weak impurity PL and produces bands at 346, 361, 381 and 402 nm. In the PL spectra of single crystals obtained from dichloroethane solution there are defect and impurity bands in the whole range of the spectra. It is shown that the purer is a single crystal, the more intense is the band at 361 nm, which can be an indicator of its purity.

The PL spectrum of the pressed stilbene polycrystal at 5 K consists of 4 bands, as in the case of a pure single crystal, only the half-width of the bands is essentially broadened and does not depend on temperature. As the temperature increases up to 300 K, the bands in this spectrum are shifted to the blue side, which is due to inhomogeneous broadening. In fact, as the temperature increases, the states of higher energy in the Gaussian distribution of the density of states will be populated. It is shown that the PL intensity of a pressed sample at 300 K is 1.5 times more intense than that of a single crystal, which is due to scattering processes in thin samples. This fact confirms that polycrysalline stilbene is the new type of effective detector.

Thermoluminescence Study of Nonisothermic Energy Transfer Kinetics to Matrix-Isolated Centers in Solid Argon

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The thermoluminescence technique is used actively for studying the localized states in crystals. Mobile electrons and holes formed as a result of exposure to any type of ionizing radiation at low temperatures are caught in traps in the course of relaxation. Heating of the sample leads to radiative electron-hole recombination of carriers released from the traps. Solid Ar with its simple crystal and electronic structures is an attractive model system suitable for fundamental research into energy relaxation and charge separation. The Cameron bands luminescence from CO-doped solid Ar was investigated using selective excitation by synchrotron radiation and thermally stimulated luminescence methods [1], the photoexcitation and TL emission spectra of the Cameron bands were measured, the activation energies and the frequency factors of charge traps were determined by numerical fitting of the TL emission spectrum [2].

We propose the analytic method of determination of kinetic parameters of electron traps thermoactivation in matrix-assisted energy transport to matrix-isolated impurity molecules in rare-gas solids. For concentration of trapped electron, n; trap filling factor $\alpha = (n_0 - n)\cdot n_0^{-1} = 1 - (n/n_0)$; heating speed $\beta = \mathrm{d}T/\mathrm{d}t$ and trap release temperature factor $\gamma = \mathrm{d}\alpha/\mathrm{d}T$ the activation energies and frequency factors of charge traps can be obtained by formulas $E_\mathrm{a} = R\dfrac{T_1T_2}{T_2 - T_1}\left(\ln\dfrac{\gamma_2}{\gamma_1} - \ln\dfrac{1-\alpha_2}{1-\alpha_1}\right)$ and $s = \beta\gamma\cdot(1-\alpha)^{-1}\exp\left(\dfrac{E_\mathrm{a}}{RT}\right)$ for two temperatures [3]. An analysis of thermoluminescence glow curves from CO-doped solid Ar confirmed the description of this curves by superposition of seven glow peaks. Calculated nonisothermal kinetic parameters are in good agreement with empirical data.

[1]. A.N. Ogurtsov. Cryocrystals Modification by Electronic Excitations. – Kharkiv: NTU "KhPI", 2009. – 368 p.

[2]. J. Becker, O.N. Grigorashchenko, A.N. Ogurtsov et al. Thermoluminescence from CO-doped solid Ar // J. Phys. D: Appl. Phys. – 1999. – V. 31. – P. 749 – 753.

[3]. O.N. Bliznjuk, A.N. Ogurtsov. Thermoluminescent Determination of Nonisothermal Kinetic Parameters of Matrix-Isolated Centers Excitation in Noble Crystals // ITE. – 2013. – N. 1. – P. 44 – 49.

Investigation of Magnetic Phase Transition in $MnPS_3$ Single Crystal by Raman Scattering

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The MPX_3 family crystals (M – transition metal, X = S, Se) continue to attract the attention of researchers in the present time. These compounds have the prominent quasi-two-dimensional properties from both – the crystalline structure as well as magnetic interactions. Interest in the magnetic properties of the MPX_3 crystals is caused by no ordinal placement of the manganese atoms forming the honeycomb structure.

The Raman spectra in the $MnPS_3$ single crystal were investigated in the frequency range of 5 – 700 cm^{-1} and in the temperature range of 5 – 300 K. Previously, this crystal was studied by Raman spectroscopy at room temperature [1,2]. In this paper, we present a novel study of the temperature dependence of Raman spectra. For the first time, for crystals of this family, the energy splitting between some of the A_g and B_g modes which previously were considered as energetically equivalent is found. There were found anomalies in the energy behavior of two low-frequency phonon modes at the phase transition of the $MnPS_3$ crystal in magnetically ordered state. Changing of frequencies of vibrational excitations at the magnetic phase transition for this crystal family was observed for the first time. Earlier, only changes of the intensities of the lines were observed at magnetic phase transition in the set of compounds. It was found, that at low temperatures two-magnon scattering spectrum has a complex form, which correlates with data obtained from absorption spectra [3].

The vibrational properties of the $MnPS_3$ crystal were calculated taking into account the LDA approximation with DFT-D (OBS) dispersion correction implemented in the CASTEP package. The calculation of phonon dispersion curves and total as well as partial densities of phonon states was carried out in the antiferromagnetic phase of $MnPS_3$ crystal. Obtained results had been compared with measured experimental spectra of Raman scattering.

[1]. Y. Mathey, R. Clement, et. al.Inorg. Chem. – 1980. – V. 19. – p. 2773 – 2779.
[2]. M.Brnasconi, G.L.Marra, et. al. Phys.Rev.B – 1988. – V. 38. – N. 17. – p. 12089 – 12099.
[3]. S.L. Gnatchenko, I.S. Kachur, V.G. Piryatinskaya, Yu.M. Vysochanskii, and M.I. Gurzan, Low. Temp. Phys. – 2011. – V. 37. – N. 2. – p. 180 – 185.

Raman and Luminescence Study of $TbAl_3(BO_3)_4$ Single Crystal

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The Raman spectra in the $TbAl_3(BO_3)_4$ single crystal were investigated in the frequency range 3 – 1600 cm^{-1} and luminescence spectra were measured in the frequency range 11800 – 21000 cm^{-1} in the temperature range of 5 – 300 K. The spectra were taken with Nd:YAG (neodymium-doped yttrium aluminum garnet) solid-state laser (λ_{exc}=532 nm) and He-Ne laser (λ_{exc}=632.8 nm). It unambiguously let us to separate Raman and luminescence spectra.

Analysis of the phonon spectrum and its comparison with the isomorphic $TbFe_3(BO_3)_4$ compound [1] were carried out. It let us to assign some vibrational modes with definite types of vibrations and find an additional line in the range of internal vibrations of BO_3 group in Raman spectra in the $TbAl_3(BO_3)_4$ single crystal. The origin of this band*is under discussion.* Using different scattering geometries, the values of splitting between the LO and TO components of polar *E* phonons were defined.

The structure of the ground multiplet $^7F_6$ of a Tb^{+3} ion in the $TbAl_3(BO_3)_4$ single crystal was investigated. The experimental values of the energies of electron transitions at 216.5, 276.0, 279.5, 440.1 and 478.0 cm^{-1} were taken from Raman data at 5 K. Upon heating up to 300 K, the experimental values of the energies of electron transitions at 213, 271, 280, 429 and 469 cm^{-1} were taken from luminescence spectra. These results are in good agreement with the data obtained by using other methods at 77 K and published in [2,3].

We studied the temperature evolution of luminescence spectra. There were found the most intensive $^5d_4 \rightarrow {}^7F_0$ transitions in the energy range of 14520 – 14660 cm^{-1}. Upon heating, the intensity of these transitions suppresses. On the other hand, the $^5d_4 \rightarrow {}^7F_6$, $^5d_4 \rightarrow {}^7F_5$ and $^5d_4 \rightarrow {}^7F_4$ transitions are not observed at 5 K. They become visible at 160 K and their intensities are comparable with intensity of Raman spectrum at 300 K. Observation of luminescence from the $^5d_4$ term (20600 – 20750 cm^{-1}) with He-Ne (15803 cm^{-1}) and solid state (18797 cm^{-1}) laser excitation indicates strong nonlinear properties of the studied crystal.

[1]. A.V. Peschanskii, A.V. Yeremenko, V.I. Fomin, L.N. Bezmaternykh, I.A. Gudim, Low. Temp. Phys. – 2014. – V. 40. – N. 2. – p. 219 – 229.
[2]. C. Gorller-Walrand, et al., Inorg. Chim. Acta, – 1987. – V. 139. p. 277 – 279.
[3]. Couwenberg, et al., Journal of Alloys and Compounds, – 1998. – V. 274. p. 157 – 163.

Investigation of the Peculiarities of the Absorbed Water on TiO_2 by NMR-Relaxation Method

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The temperature dependence of the spin-lattice relaxation time (SLR) for protons of absorbed water on the surface of the TiO_2micro-sphere in the temperature range 170 – 400 K has been investigated. It was shown that in investigated temperature range there are two mechanisms of SLR: low-temperature (170-280 K) and high-temperature (300-400 K). The obtained data evidence of the fact that two types absorbed molecules of water on the TiO_2surface exists: more active with E_{a1}=3.9 кJ/mol and less mobile with E_{a2} = 6.7 кJ/mol. This can be explained by different position of absorbed molecular groups of water on the surface of the TiO_2micro-sphere.For the free (non-interacting) water, where mechanism of SLR completely determined by hydrogen bond dynamics, the two values of the activation barriers was obtained: E_{a1} = 16 кJ/mol and E_{a2} = 20 кJ/mol. These barriers correspond to the energy of the distorted and undistorted hydrogen bonds.The comparison presented values E_a show that for the absorbed water barrier E_a more in four times less then for the pure water. The correlation time τ_c was calculated for the low-temperature region of relaxation with E_{a1} = 6.7 кJ/mol. It was obtained that τ_c value severely less then corresponding value for free molecules water. This can be explained by influence TiO_2 surface on dynamics of the bounded hydrogen atoms of the absorbed water.

It is necessary to note that distances between oxygen atoms of the TiO_2 micro-sphere, which form the hydrogen bonds are short. Therefore the distances between corresponding minima of the potential energy for the absorbed protons are small. This must lead to decreasing of the value potential barriers and confirm by obtained experimental results. The next layer forms H-bonds between oxygen atoms of the absorbed water and oxygen atoms of the free water of the next layer. Thus the “expressiveness” of the potential relief increases with increase of the wide of water on surface of the TiO_2 micro-sphere. However obtained values $E_{a,}$, which characterize state of the protons, do not reach to value for free water. Besides a strong interaction of the absorbed water with the TiO_2 micro-sphere lead to degreasing of velocity proton migration in the absorbed water.

Optical Studies of Phase Transitions and Absorption Edge in Cu_6PS_5Br-Cu_7PS_6Mixed Crystals

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Cu_6PS_5Br crystals belong to the family of compounds with argyrodite structure. At room temperature Cu_6PS_5Br crystals belong to the cubic syngony ($F\bar{4}3m$space group) while at low temperatures two phase transitions (PTs) occur: a ferroelastic one at T_{II} =(268±2) K and a superionic one at T_I=(166–180) K. Below the ferroelastic PT temperature Cu_6PS_5Brcrystals belong to the monoclynic syngony (*Cc* space group), and the superionic PT reveals the features of an isostructural transformation. In Cu_7PS_6 a PT is observed at 515 K from the high-temperature phase with $F\bar{4}3m$ symmetry to the low-temperature phase with $P2_13$ symmetry. Here we present results of the isoabsorption and polarization studies of PT as well as the absorption edge studies in $(Cu_6PS_5Br)_{1-x}(Cu_7PS_6)_x$mixed crystals.

$(Cu_6PS_5Br)_{1-x}(Cu_7PS_6)_x$mixed crystals were grown by chemical vapour transport technique. It is shown that at $x\leq0.2$ in $(Cu_6PS_5Br)_{1-x}(Cu_7PS_6)_x$mixed crystals the solid solutions based on Cu_6PS_5Br with $F\bar{4}3m$ symmetry are obtained. Isoabsorption, polarization and absorption edge studies were carried out in the temperature range 77–320 K. On the isoabsorption curves in the range of ferroelastic second-order PT a specific knee is observed that is smeared with increase of Cu_7PS_6 content in $(Cu_6PS_5Br)_{1-x}(Cu_7PS_6)_x$mixed crystals.Polarization studies have shown that at PT at $T=T_{II}$ the light transmission in the polarizer-crystal-analyzer system is observed. This PT is accompanied by the transition from isotropic paraelastic phase to anisotropic ferroelastic phase.As a result of isoabsorption and polarization measurements the dependence of ferroelastic PT temperature on Cu_7PS_6 content in $(Cu_6PS_5Br)_{1-x}(Cu_7PS_6)_x$crystals is obtained. It is shown that the increase of Cu_7PS_6 content leads to decrease of the PT temperature at $T=T_{II}$from 265.6 K in Cu_6PS_5Br crystal to 255 K in $(Cu_6PS_5Br)_{0.9}(Cu_7PS_6)_{0.1}$mixed crystal. Temperature studies of $(Cu_6PS_5Br)_{1-x}(Cu_7PS_6)_x$mixed crystals have shown that at $T>T_I$, exponential parts appear at the absorption edge, the behavior of which is described by the Urbach rule.Temperature dependences of the absorption edge steepness parameter are well described by Mahr formula.At Cu_7PS_6 content increase the enhancement of exciton-phonon interaction in $(Cu_6PS_5Br)_{1-x}(Cu_7PS_6)_x$mixed crystals is observed.It is revealed that with increase of Cu_7PS_6 content thecontribution of sum of structural and compositional disordering as well as the contribution of temperature disordering in $(Cu_6PS_5Br)_{1-x}(Cu_7PS_6)_x$ mixed crystals is increased.

Luminescence Spectra of Benzoxazoles Undergoing Excited State Proton Transfer in Solid State

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2,5-bis(2-benzoxazolyl)phenol (DBP) and 2,5-bis(2-benzoxazolyl)hydroquinone (BBHQ) are luminescent benzoxazole derivatives undergoing photoinduced excited state intramolecular proton transfer [1]. In the ground state the molecules of BBHQ and DBP have enol structures with OH…N hydrogen bonds. Upon the proton transfer the keto structure with an O…HN hydrogen bond is formed exhibiting a fluorescence band with an anomalously large Stokes shift. The luminescence and absorption spectra of DBP and BBHQ were measured for polycrystalline powders and solutions in nonpolar solvent.The luminescence spectra of solid-state DBP and BBHQ were found to comprise bands with normal and anomalously large Stokes shifts. The quantum chemical calculations demonstrate that the energies of the enol and keto forms in the first excited singlet state differ much less than in the ground state and the dual fluorescence is caused by existence of the enol and keto forms in the first excited singlet state. The bands with the normal Stokes shift are assigned to the excited enol forms of the molecules, the bands with the large Stokes shift are assigned to the keto forms. BBHQ in the solid state demonstrates the keto fluorescence band similar to one observed in solution with a small red shift by 0.03 eV, while DBP exhibits change of the shape and position of the band originated from the keto form.

[1]. J.M. Kauffman and G.S.Bajwa. Synthesis and photophysical properties of fluorescent 2,5-dibenzoxazolylphenoles and related compounds with excited state proton transfer // J. Heterocyclic Chem. – 1993. – V. 30. – p. 1613 – 1622.

Raman Scattering on Low-Frequency Vibrations of Crystalline 2-(2’-hydroxyphenyl)benzoxazole

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2-(2‘-hydroxyphenyl)benzoxazole (HBO) is a compound that exhibits excited state intramolecular proton transfer. Photoinduced excited state intramolecular proton transfer has attracted attention of researchers for several decades as an ultrafast photochemical reaction and a process that could be utilized for a number of applications including laser dyes and electroluminescent materials. Low-frequency intramolecular vibrations were considered to play a prominent role in the proton transfer process changing the distance between the proton donor and acceptor in the molecule of HBO [1]. In molecular crystal, intermolecular forces cause the appearance of vibrational motions corresponding to translational and rotational degrees of freedom of the molecule. The frequencies of these external translational and librational vibrations are usually in the range of 0-150 cm^{-1} and new lattice modes considered as mixing of internal and external vibrations could appear. Unpolarized Raman spectrum of crystalline 2-(2‘-hydroxyphenyl)benzoxazole in the region 15-350 cm^{-1} is compared with the results of semi-empirical lattice vibration calculations and oriented gas model. Raman bands observed in the range 25-95 cm^{-1} are assigned to vibrations that are predominantly external, bands with frequencies above 150 cm^{-1} are attributed to internal vibrations. The molecular in-plane bending vibration that changes distance between oxygen and nitrogen atoms constituting the proton transfer site undergoes splitting and mixing with out-of-plane and external vibrations giving rise to the Raman bands observed at 116 and 141 cm^{-1} [2].

[1]. M. Pfeiffer et al. Analysis of the Vibrational Spectra of Heterocyclic Aromatic Molecules Showing Internal Proton and Deuterium Transfer // J. Raman Spectrosc. – 1997. – V. 28. – p. 61 – 72.

[2]. Y. Syetov. Low-frequency Raman spectrum of crystalline 2-(2’-hydroxyphenyl)benzoxazole and DFTB phonon calculations // Ukr. J. Phys. Opt. – 2017. – V. 18. – p. 67 – 76.

About the Features of Formation of Radiation Defects in the Diode Structures with Impurities of Rare Earth Elements

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It is known that the main part of the impurities of rare earth elements (REE) in silicon is electrically neutral and at the same time their presence has a significant influence on the thermal processes of radiation defect formation and ultimately on the electrical properties of doped silicon [1-2]. However, in the literature there is no consensus about the electrical activity of the impurities of REE and their interaction with thermal (TD) and radiation defects (RD), as well as other impurities in silicon.

In this work, the results of complex researches of processes of defect formation in silicon, doped with rare earth elements. As the samples used were n-Si doped with erbium in the process of growing, control samples were the samples grown n-Si with identical electrical parameters. From measurements of the spectra of nonstationary capacitance spectroscopy of deep levels (DLTS) of the samples n-Si<Er>, established that the atoms of erbium do not form deep levels in the bandgap of the base region of the structures of the Au-Si<Er>-Sb, although their total concentration in the silicon volume according to neutron activation analysis is 10^{16}-10^{18} cm^{-3}.

Consider the results of studies of the effect of γ-irradiation on the properties of Si with impurities of REE on n-Si<Er> with different contents of Er and interstitial oxygen. Analysis of DLTS spectra shows that as a result of irradiation in the samples n-Si<Er> (N_o^{opt} ˜$8\cdot10^{16}$ cm^{-3}) formed a new DL with an ionization energy of E_c- 0.17 eV, its parameters coincide with the parameters of known RD – A-center (the complex vacancy–oxygen). In samples with N_o^{opt} ˜$8\cdot10^{17}$ cm^{-3} observed 2 new DL: E_c-0.17 eV and E_c-0.43 eV, and the dominant is the second DL, the parameters of which coincide with the parameters of another famous RD – E-center (the complex of vacancy – phosphorus). Add that the A - and E - centers are observed also in the control samples Si (without Er).

Comparison of the dose dependencies observed deep levels in irradiated.

n-Si<Er> the same dependencies in the control samples shows that the rate of introduction of RD in samples containing erbium, significantly lower than in the control. Thus, the presence of Er atoms into Si reduces the effectiveness of education RD.

[1]. Milwidsky M.G., Karpov Yu., Turov B.M., Voronkov V.V., Kovaleva T.A., Moscow, "Science". 1985. Doped semiconductor materials. S. 97.

Spectra NQR I^{127} Mixed Layered Semiconductors

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In this work the temperature dependence of the parameters of the NQR spectrum of the layered semiconductor crystals $(BiI_3)_{(1-x)}(PbI_2)_x$ and $Pb_{x-1}Cd_xI_2$ have been studied. The results of research of the concentration and temperature dependences of the NQR spectrum parameters of I^{127} mixed layered semiconductors $Pb_{x-1}Cd_xI_2$ and $(BiI_3)_{(1-x)}(PbI_2)_x$are presented for $x \leq 0{,}30$ and 77-150 K. It is shown that at low content $x \leq 0{,}08$ PbI_2 for $(BiI_3)_{(1-x)}(PbI_2)_x$ and $x \leq 0{,}02$ CdI_2 for $Pb_{x-1}Cd_xI_2$ temperature coefficient of NQR frequency does not undergo significant changes, indicating the conservation the quasi-two-dimensional nature of the vibrational states. For BiI_3 crystals at 77K with PbI_2 contents of x=0,20 and 0,3, a line ν′ was observed in the I^{127} NQR spectrum the parameters of which differed significantly from the parameters of the I^{127} line ν for pure BiI_3 (Fig. 1). The temperature coefficients of the frequency ($d\nu/dT$) increased in comparison with the line ν′ for this new line ν in the NQR spectrum. As a result, can be done the conclusion that, at the PbI_2 content range $0{,}2 \leq x \leq 0{,}6$ compared with range $0 \leq x \leq 0{,}08$ the degree quasi two dimensional of phonon spectrum becomes different (spectrum becomes more ‘softer’).

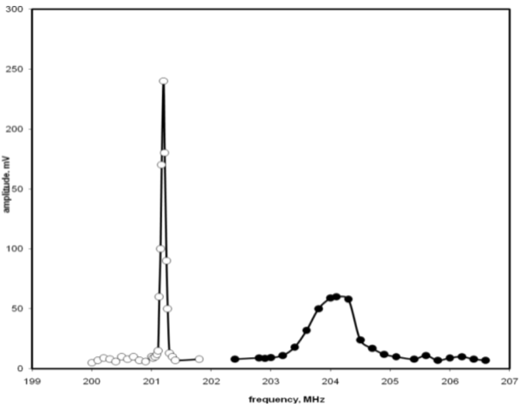

Fig. 1. NQR spectra I^{127} for $(BiI_3)_{(1-x)}(PbI_2)_x$ (±3/2↔±5/2) at T=77 K: ○ – for x=0 (ν=201,2 MHz), and ● – for x=0,2 (ν_1=204,150 MHz - new line).

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Liquid Crystals

^{1}H NMR Study of Lyotropic Liquid Crystals with Biomedical Interest and Metabolites in Water Solutions

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Lyotropic liquid crystals and liquid crystalline gels feel a certain renaissance attracting a considerable attention in areas of biomaterials, electrooptics and as templates for the preparation of mesoporous materials and ordered thin films [1,2]. Aqueous solution of lyotropic liquid crystals can serve as perfect model systems in biomedical research studying biological- and life mater important structures and their evolution upon the external action of temperature or reacting environments.

In the present work, the liquid crystalline phases that are formed in disodium cromoglycate and Sunset yellow in water solutions were studied applying ^{1}H NMR spectroscopy. The borders between nematic (N), coexisting nematic (N) and hexagonal (M) and completely hexagonal phases were detected analyzing ^{1}H chemical shifts and their signal widths varying concentration and temperature. The results were compared with the related ^{1}H and ^{2}H NMR data [3].

In parallel water and deuterated water solutions of different pH (from 5.5 to 7)containing different metabolites were prepared and their ^{1}H NMR spectra were analyzed. These data can be used recognizing metabolites in various phases.

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[1]. G. H. Brown, J. J. Wolken, *Liquid Crystals and Biological Structures*, Academic Press, New York, 1979. 187 p.
[2]. H. E. Schaefer, *Nanoscience. The Science of the Small in Physics, Engineering, Chemistry, Biology and Medicine*, Springer-Verlag, Berlin, Heidelberg, 2010, 772 p.
[3]. E. Troche-Pesqueira, M. M. Cid, A. Navarro-Vázquez, Org. Biomol. Chem. **12**, 1957 (2014).

Director Orientation Instability in Homeotropic Nematic Liquid Crystal Cell in Electric Field

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Orientation instability of director in the cell containing nematic liquid crystal with negative dielectric anisotropy placed in external static electric field was investigated. We considered the gliding of an easy axis in the plane perpendicular to one of the polymer substrates of the cell.

The gliding is explained by reorientation of elastic fragments of the polymer molecules on the cell substrate, which is a result of the interaction of their permanent or induced dipole moments with electric field. The corresponding contribution from the interaction to the free energy of the system was taken to be linear by electric field for permanent dipole moments unlike the case of induced dipole moments where the additional term was assumed to be quadratic by electric field.

It was shown that the orientation instability has threshold behavior which does not depend on the character of the interaction of the easy axis with electric field. The evolution of nematic director and easy axis and their relaxation after switch off the voltage were analyzed in both cases of the interaction. Calculated time dependence of deviation angle of the easy axis was compared with data taken from experimental papers.

Cooling Rate Effect on 5CB Liquid Crystal Luminescence Spectra

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Recently, the luminescence properties of cyanobiphenyls homologous series, including liquid crystal (LC) 5CB, have been investigated in solvents of different nature, in its isotropic state and mesophase modifications [1-3]. Information about the systematic experiments on 5CB luminescence at low temperatures ($\leq$ 77 K) is absent in publications [4]. The effect of cooling rate on LC spectral properties which can be substantially depended on this factor is practically remained unstudied.

We have found that peculiarities of 5CB LC luminescence spectrum, measured at 4.2 K, essentially depend on the sample cooling rate at temperature decrease from the room to helium ones. This effect was studied at the rates of 200°/min. ("fast cooling") and 5°/min. ("slow cooling").

We have determined that under fast cooling the luminescence spectrum consists of a single broad structureless band with $\lambda_{max} \approx 360$ nm. Under slow cooling the band maximum shifts to the "red" side (towards high wavelengths) on ~ 30 nm and its halfwidth decreases by 20%. A new clearly seen structured band with $\lambda_{max} \approx 378$ nm appears at the short-wave edge of the luminescence spectrum.

A graphical separation of luminescence bands was performed in the cases of both cooling rates. Based on the data analysis, the suggestion was made that the effect observed could be caused by different ratios of monomer and dimer emission centers realized in the material under fast or slow cooling.

The role of the LC glassy phase which can be formed under fast sample cooling [5-6] is discussed for the studied effect.

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[1]. J.I. Kukielski. // J. Mol. Struct. – 1998, – V. 1–8, – p. 478

[2]. A.M. Klock, W Retting, J. Hofkens, M. van Damme, F.C. Schryrer. // J. of Photochem and Photobiol. – 1995, – V. 85, – p. 11

[3]. T. Ikeda, S. Kurihara, S.Taruke. // J. Phys. Chem. – 1990, – V. 94, – p. 6550

[4]. T. Bezrodna, V. Melnyk, V.Vorobjov, G. Puchkovska. // J. Lum. – 2010, – V. 130, – p. 1134

[5]. В.А. Бернштейн, В.М. Егоров Дифференциальная сканирующая калориметрия в физикохимии полимеров. Ленинград, «Химия», –1990, – стр. 46 – 56

[6]. N.A. Davydova, V.I. Melnik, J. Baran, M. Drozd. // J. Mol. Structure. – 2003, – V. 651–653, – p. 171– 175

Dispersions of Anisometric Nanoparticles in Cholesteric Liquid Crystals: Comparison of Carbon Nanotubes and Laponite Platelets

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In our recent papers [1, 2], we reported various peculiar features that could be observed (by changes in optical transmission and optical microscopy studies) when carbon nanotubes (CNT) were dispersed in cholesteric liquid crystals (CLC). On the level of supramolecular organization, at low concentrations the introduced CNT tended to concentrate on CLC defects (e.g., oily streaks), while at higher concentrations the nanotubes formed aggregates of their own, with oily streaks disappearing.

Since introduction of micro- and nanoparticles of different kinds to liquid crystal matrices is a topical direction of numerous studies, we tried to determine how substitution of CNT by particles of different anisometry would affect the observed properties under the same experimental conditions.

In our studies, we used samples of organomodified laponite, when exfoliated laponite platelets would be dispersed in the orientationally ordered liquid crystal matrix. In particular, we used two types of laponite samples obtained by different preparation procedures (so-called ‘hot” and “cold” laponite).

Two main conclusions could be made; (1) the laponite particles appeared to be dispersed with higher or lower degree of homogeneity in all the concentration range, without any clear signs of interaction with CLC defects, and (2) “cold” laponite clearly showed signs of better exfoliation, which was reflected in optical transmissions, on microphotographs obtained with optical microscope, and in differential scanning calorimetry thermograms obtained in the vicinity of nematic (cholesteric) to isotropic phase transitions, both on heating and cooling.

As an additional result that could be useful from the standpoint of possible applications, one could note that simultaneous introduction of CNT and exfoliated laponite particles substantially improved the homogeneity and time stability of the obtained nanomaterials.

[1]. L.N.Lisetski, S.S.Minenko, A.N.Samoilov, N.I.Lebovka. Optical Density and Microstructure-Related Properties of Photoactive Nematic and Cholesteric Liquid Crystals with Carbon Nanotubes // Journal of Molecular Liquids. – 2017. – V. 235. – N. 1. – p. 90-97

[2]. A.N.Samoilov, S.S.Minenko, L.N.Lisetski, M.S.Soskin, S.I.Torgova, N.I.Lebovka. Anomalous optical properties of photoactive cholesteric liquid crystal doped with single-walled carbon nanotubes // Liquid crystals. – 2017. – DOI: 10.1080/02678292.2017.1314560

Photoinduced Freedericks-Type Transition in Carbon Nanotube-Doped Nematic Mixtures

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Development of various electrooptical, optoelectronic and sensor devices based on reorientation of liquid crystal (LC) structures under electric fields and other external factors is a topical direction of modern research and technology. New possibilities are offered by introduction of various micro- and nanoparticles into LC matrices.

In our study, we used nematic mixtures based on nematic cyanobiphenyls (e.g., 5CB) and photosensitive azoxy nematics (in which *trans-cis* isomerization under UV irradiation could lead to easily detectable changes in optical properties). Appropriate optimization of the LC composition allowed us to combine possibilities of voltage-induced Freedericks-type transition and sensitivity to UV irradiation. Under application of a pre-threshold basic bias voltage, conditions for realization of UV-induced transition from planar to homeotropic orientation have been established. In a specific variant, threshold voltages of the Freedericks-type transition could be lowered by preliminary UV irradiation of the LC cell.

The planar to homeotropic transition could be monitored both by optical transmittance in standard geometry with polaroids and by changes in electric conductivity. In the latter case, the recorded response could be substantially increased when carbon nanotubes were dispersed in the LC matrix.

Prospects of possible applications of the observed effects are discussed, including UV sensors, circuit elements with variable capacitance, attenuators for high-frequency electromagnetic fields, etc. Several possibilities are proposed to increase the time stability of LC active materials with carbon nanotubes, including induction of helical twisting and addition of particles with different anisometry.

Improved Conformal Mapping Technique for Calculating Plane Director Profiles in Nematic Cells

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We propose an improved conformal mapping technique for analytical calculation of two-dimensional director profiles in a nematic liquid crystal (NLC) cell. We consider the case of the strong anchoring and the piecewise constant director pretilt on the piecewise smooth substrates which bound the cell. Obtained expressions for the director profile explicitly depend on the conformal mapping which maps the cross-section region of the cell onto the upper half plane of a complex plane. An advantage of our method in comparison with the standard conformal mapping technique is that it does not require the knowledge of the inverse mapping and the calculation of the integral in the Poisson formula. The proposed technique allows one to take into account topological defects in the bulk of the NLC on the symmetry axis of the cross-section region. As an example of how the method can be used, we find an analytical expression for the director profile in a horizontal cylindrical groove partly filled with the NLC. We consider the case where a disclination line parallel to the axis of the groove occurs in the bulk of the NLC. The equilibrium position of the disclination line is found as a function of the height up to which the groove is filled.

Comparative study of Provitamin D Photoisomerization in Solutions and in Liquid Crystalline Matrices by UV Absorption Spectroscopy

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Photoisomerization of Provitamin D_3 (7-dehydrocholesterol, 7-DHC), - the initial stage of Vitamin D_3 synthesis, - was investigated in solutions with polar and nonpolar solvents and in a number of liquid crystalline matrices using UV absorption spectroscopy. As is known, UV irradiation of 7-DHC within its absorption band (240–315 nm) leads to the formation of a conformationally flexible molecule of previtamin *D*which is further converted into Vitamin D_3 via thermo-induced intra-molecular *H* shift.

However, Previtamin D_3 is UV-unstable and undergoes a series of UV-induced photoconversions, which lead to the formation of a multicomponent photoisomer mixture. Since the quantum yield of *cis-trans* isomerization is high (0.48) and the extinction coefficient of the *trans*-isomer Tachysterol is significantly higher than that of all others, the increase in the absorbance under UV irradiation reflects the efficiency of Tachysterol accumulation.

When investigating solutions, it was found that the polarity of the solvent negligibly affects the efficiency of *cis-trans* isomerization, and no effect of the 7-DHC concentration on the Tachysterol formation was found [1].

A completely different situation was observed in the nematic LC matrix, where dissolution of the chiral 7-DHC molecules led to the induction of the cholesteric phase, and the increase in 7-DHC concentration was accompanied by the cholesteric helix twisting, i.e. reduction of its step [1].

Interestingly, in viscous LC medium significant increase in the efficiency of *cis-trans* isomerization with the increase of 7-DHC concentration was found in both nematic and cholesteric LCs [1,2]. At the same time with an increase in mesophase temperature this effect reduced up to the disappearing of the 7-DHC concentration dependence in the isotropic phase. Altogether, our results indicate the collective character of *cis–trans* isomerization in liquid crystals due to the medium ordering, and the spectral kinetics of provitamin *D* photoisomerization can serve as a highly sensitive intrinsic probe of structural ordering of an induced cholesteric LCs.

[1]. O.G. Dmitrenko, I.P. Terenetskaya and W.Reischl. Solvent effect on previtamin D conformational equilibrium and its photoreactions // J. Photochem. Photobiol. A:Chemistry. – 1997. - V.104. - p. 113 - 117.

[2]. T.N. Orlova, I.P. Terenetskaya.Specific features of photoisomerization of provitamin D_3 in a nematic liquid crystal. // Optics and Spectroscopy – 2006. – V.100. – p. 584 - 589.

Thermal and Spectroscopic Characterization of Confined Hydrogen-Bonded Liquid Crystals

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The aim of the present study was to investigate a new class of LCs - hydrogen-bonded LCs (HBLC) confined to mesoporous MCM-41 molecular sieves. Despite fundamental reasons and their applicative properties the molecular dynamics of HBLC liquid crystals confined in inorganic porous matrices are much less studied than that of the related series of cyanobiphenyls. Here we focused on the two commercial HBLC mixtures (CC-3 and PC-29) comprising several members of *n*-alkylbenzoic CH_3-C_nH_{2n-2}-C_6H_5-COOH (*n*-ABA, *n*=3,4,5) and *m*-alkylcyclohexane carboxylic CH_3-C_nH_{2n-2}-C_6H_{11}-COOH (*m*-ACHA, *m*=2,4,5, PC-29) serieswith three to five carbon atoms in the alkyl tail confined in nanoporous MCM-41 molecular sieves (cylindrical pores about 4 nm in diameter). The molecular dynamics and thermotropic properties of the confined HBLC were investigated with differential scanning calorimetry (DSC) and Fourier transformed infrared spectroscopy (FTIR). A Perkin-Elmer Model DSC7 equipped with a refrigerated cooling unit CCA-7 was used for DSC measurements in the temperature interval of 20-150 °C with the heating and cooling rate of 8 °/min. FTIR spectra (4000-380 cm^{-1}) were measured in the 23-180 °C temperature range using Bruker IFS-88 spectrophotometer with 2 cm^{-1} resolution. The data are compared with those previously obtained on pure *4*-ABA and *6*-ACHA compounds [1]. It is shown that phase behavior of the HBLC confined to MCM-41 significantly differs from that observed in a bulk material, divergence being related to both surface interactions and geometrical constraints. With-variable-temperature FTIR spectroscopy it is shown that the confined HBLC are thermally stable up to 150 °C. Considering that the alkylbenzoate materials have electro-optical properties, this class of composite nanomaterials seems especially interesting for their potential applications in microelectronics, optical devices, magnetic materials and chemical recognition.

[1]. I. Gnatyuk, T. Gavrilko, O. Yaroshchuk, N. Holovina, N. Scherban, J. Baran, and M. Drozd. *J. Molec. Struct.* 1126 (2016) 19-28.

Dye Doped CLC-Lasers: Interdependence of Spectral and Angular Characteristics of Lasing

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Lasers on dye-doped cholesteric liquid crystals (CLC) [1] are studied intensively with the aim of improving their options for further application. In the present work, the spectral and spatial characteristics of lasing emission with changing the mutual orientation of directors on the orienting substrate were investigated.

For given CLC on a ternary mixture of cholesterol esters, activated phenolenone dye F490 it was established, that parallel orientation of directors provided lasing with lowest thresholds. The spectrum of this radiation was presented by three longitudinal modes with small changes under practically available optical pumping. The origin of the ring structure of a laser beam is studied, and it is established that transverse this structure is presented on some higher Laguerre-Gauss modes.

When orthogonal orientations of directors took place the oscillation threshold increased approximately 1 order, however, the lasing spectrum consisted of the main longitudinal mode of the cavity in a wide range of pump energies. Higher transverse mode in the spatial pattern of radiation already did not excited. It was also found that similar effect is observed only for a certain type of orienting substrates.

The results can be explained by the influence of the defect of CLC helical structure type "phase jump" [2], which can occur in such a viscous medium and affects the lasing spectra. A shift of the lasing spectrum and an increase in the lasing threshold under such conditions can testify to the presence of a defect in such structure, though no dip in the spectrum is registered. We are exploring the possibility of existence ofsuch a defectin theselective reflectionbandof the CLC.

The lasing peculiarity of CLC with isotropic layer in photon cavity were studied.

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[1]. Ilchishin, and E. Tikhonov. Progress in Quantum Electron. - 2015. -V. 41. - p. 1 - 22.
[2]. V. Belyakov, and S. Semenov. JETP.- 2011.-V.112. -p. 694 -706.

Patterns in Liquid Crystals Induced by (AC+DC) Electric Fields

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A nematic liquid crystal (NLC) shows an orientational order which is characterized by a director, **n(r).** The director can be re-oriented by an applied electric field. This distortion is a basic physical effect for several electro-optical devices. Application of the electric field also induces spatially periodic patterns in NLC films [1]. Thus, both theoretical and experimental studies have been concentrated on pattern forming phenomena obtained by electric fields [2]. In this study, we present the experimental results on electroconvection patterns induced by combined ac and dc voltages of different frequency and amplitude values [3,4]. Experimental observations were performed with planar aligned NLC film sandwiched between two transparent electrodes. The voltage-induced patterns were observed and recorded by using a polarizing microscope with a digital camera. The electroconvention patterns with different morphologies were obtained at superposed ac and dc voltages. It was found that the superposition of voltages inhibits the pattern forming mechanism. Therefore, the patternless region extends to much higher voltages. The obtained experimental results were compared with the theoretical predictions.

[1]. Á. Buka, N. Éber, W. Pesch, L. Kramer: Convective patterns in liquid crystals driven by electric field. In. *Self-Assembly, Pattern Formation and Growth Phenomena in Nano-Systems.* Eds. A. A. Golovin, A. A. Nepomnyashchy, NATO Science Series II, Mathematics, Physics and Chemistry, Vol. 218, Springer, Dordrecht, 2006, pp. 55-82.

[2]. Á. Buka, T. Tóth-Katona, N. Éber, A. Krekhov and W. Pesch, Chapter 4. The role of flexoelectricity in pattern formation. In *Flexoelectricity in Liquid Crystals. Theory, Experiments and Applications.* Eds. Á. Buka and N. Éber, Imperial College Press, London, 2012, pp. 101–135.

[3]. Krekhov, W. Decker, W. Pesch, N. Éber, P. Salamon, B. Fekete, Á. Buka, *Patterns driven by combined AC and DC electric fields in nematic liquid crystals*, Phys. Rev. E 89 052507 (2014).

[4]. N. Éber, P. Salamon, B. A. Fekete, R. Karapinar, A. Krekhov, and Á. Buka, *Suppression of spatially periodic patterns by dc voltage*, Phys. Rev E 93, 042701 (2016).

Capacitance-Voltage Characteristics of a Ferroelectric Liquid Crystal

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Capacitance characteristics of a liquid crystal film can usually be used to determine dielectric and elastic constants of the liquid crystal material [1]. Capacitance of ferroelectric liquid crystal (FLC) is also important research topic due to device applications [2,3]. In this study, frequency-dependent capacitance-voltage (C-V) characteristics of a surface stabilized FLC film were studied. The experimental measurements were carried out by measuring the capacitance while varying the AC signal voltage applied to the FLC film. C-V measurements were taken at room temperature. Frequency was also varied between 1 kHz and 1 MHz to measure capacitance across a wide frequency range. There is a hysteresis in plots of C-V loops. In the C-V characteristics curves the height of the peaks decrease with increasing frequency due to director orientation of FLC molecules. The capacitance also decreases with increasing frequency. The experimental results were also compared with a theoretical model.

[1]. Y. Wen-Jiang et al. Determining the sum of flexoelectric coefficients in nematic liquid crystals by the capacitance method, Chin. Phys. B, 23, 116101 (2014).

[2]. M. Rahman et al. Frequency-dependent capacitance-voltage hysteresis in ferroelectric liquid crystals: An effect of the frequency dependence of dielectric biaxiality, J. Appl. Phys. 98, 024114 (2005).

[3]. J. R. Daniel et al. Experimental observation of negative capacitance in ferroelectrics at room temperature, Nano Lett., 14, 3864 (2014).

Ultra-Fast Optical Response of Stressed Liquid Crystal Systems

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The principal problem of the existing liquid crystal (LC) optical elements is their relatively slow response to an electric field, which is rarely less than 0.1 s. At the same time, very often a much faster response is required. The problem of fast response can be solved by using stressed liquid crystals (SLC) formed in polymer matrix which is oriented by mechanical shearing [1].

In this work, we investigate the effect of the polymer concentration and the shear magnitude on the switching characteristics of SLC based on LC 5CB with polymer NOA65 by Norland. The switching-on time were 150-500 μs (depending on the applied voltage) for SLC composition and cell thickness of 11 μm. The switching-off times became as low as 1 ms for maximal shear distance (Fig. 1). Thus, the switching characteristics of the SLC compositions significantly exceed the characteristics of an ordinary nematic LC and SLC materials demonstrate great potential for application in fast LC optical elements.

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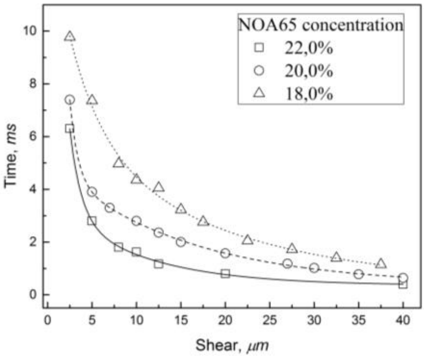

Fig. 1. Dependence of the switching-off time on the shear magnitude for different concentration of the polymer in SLC mixture.

[1]. J.L.West, G.Zhang, A.Glushchenko and Yu.Reznikov // Appl.Phys.Lett. – 2005. – N. 86. – p. 031111.

Two-dimensional Equilibrium Configuration of Nematic Liquid Crystal Director inside a Circular Cylinder

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We propose an analytical method to calculate the two-dimensional equilibrium configuration of director field of nematic liquid crystal in a simply connected domain with given piecewise pretilt of director at the boundary. The proposed method takes into account the presence of the topological defects of the structure of director field within the considered two-dimensional area. The analytical approach is based on the method of conformal mapping but does not require calculating the Poisson integral at the result. We used the proposed method to obtain two-dimensional equilibrium configurations of the director field of nematic liquid crystal inside a horizontal right circular cylinder. The easy axis orientation at the one arc of the circle of cylinder cross section was considered to be homeotropic. The easy axis has planar orientation at the rest of the circle and lies in the plane of cylinder cross section. The anchoring energy of liquid crystal with inner side of cylinder surface is infinite. We considered the case with disclination line of strength $+1/2$, which appeared in nematic bulk parallel to the axis of the cylinder. Using the approximation of plane deformations, we obtained an analytical expression for the director field in the nematic bulk. The equilibrium distance between the disclination line and cylinder axis was calculated. The dependence of the distance on the central angle α of the arc of the cross-section circle with homeotropic director orientation was investigated. Interval of values of the angle α, for which there are two possible locations of the disclination line in the nematic bulk, was established. For other values of the central angle α there is only one location of the disclination in the nematic bulk.

Director Orientation Instability of Nematic Liquid Crystal in Homeotropic Cell with Tunable Boundary Conditions

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Reorientation of nematic director in homeotropic cell in external static electric field was investigated. Nematic liquid crystal has positive dielectric anisotropy and applied electric field is parallel to the cell substrates. We considered the gliding of an easy axis in the plane perpendicular to one of the polymer substrates of the cell.

The gliding occurs due to reorientation of elastic fragments of the polymer molecules on the cell substrate, which is a result of influence of electric field on their permanent or induced dipole moments. The additional term in the free energy expression, which describes the coupling of easy axis and electric field, is assumed to be linear or quadratic by electric field for permanent or induced dipole moments respectively.

The orientation instability can arise under applied voltage higher than some threshold value or cannot show such behavior, which depends on the character of the easy axis – electric field coupling. Remarkably that the threshold voltage is more than two times smaller in comparison with the case of Freedericksz transition with the strong anchoring on both substrates. The temporal behavior of nematic director and easy axis was investigated in both cases.

Birefringence Dispersion of the Small-Molecule Liquid Crystalline Layers in External Fields: Applications to Interferential Polarization Filters

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The molecules that are preferentially oriented on a direction which involves an advanced degree of orientation order, but a low degree of positional order can be organized in nematic liquid crystals. The preferential direction of the long axes can be easily modified by external factors, such as electric of magnetic fields, temperature, or surface interactions. It was noticed by optical analysis of the nematic mesophases that an ideal balance configuration is indicated by a transparency close to 100%. MBBA – N-(p-methoxy-benzylidene)-p-butylaniline – shows nematic phase within 20-40°C, it is more accessible in applications.

MBBA is a uniax liquid crystal with two values of the refractive index for ordinary and extraordinary rays whose difference determines its birefringence, an optical parameter strongly dependent on the external electric field. A series of results for measurements in absence and in the presence of external electrostatic fields are discussed here related to the applications to interferential polarization filters made by MBBA.

Dielectric Spectra and Development of Electric Percolation in the Nematic Liquid Crystal Suspensions of Carbon Nanotubes

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Using oscilloscope method [1], dielectric spectra of nematic liquid crystal (LC) 5CB filled with multiwalled carbon nanotubes (CNTs) (Fig. 1) were measured in a very broad range of CNT concentrations (C_{NT}=10^{-5}-2.5 wt %).

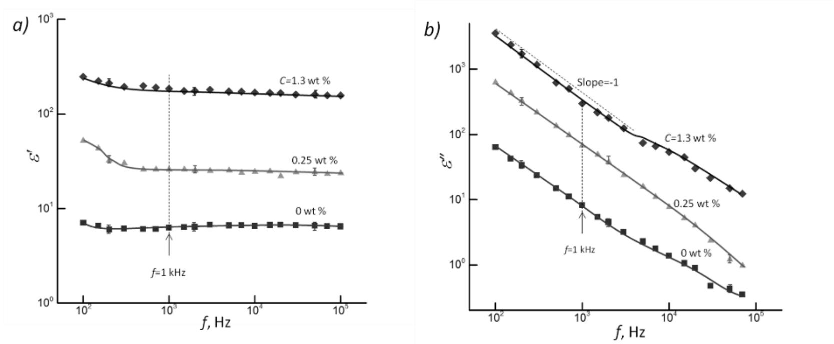

Fig. 1. Frequency dependences of the real ε' (a) and imaginary ε'' (b) parts of the complex dielectric constant of 5CB-CNTs suspensions at three different concentrations of CNTs: 0, 0.25 and 1.3 wt%.

The obtained data were used to determine concentration dependences of conductivity $\sigma(C_{NT})$ and dielectric constant, $\varepsilon'(C_{NT})$. Several stages in the development of electrical percolation correlated with the stages of structural evolution were determined. Initial quasi-linear part I ($C_{NT}<10^{-4}$ wt%) can be assigned to charge transfer by single NTs (Maxwell mechanism). In concentration range II (C_{NT}=10^{-4}-10^{-3} wt%) the electrical conductivity σ only slightly grows with C_{NT}. It can reflect formation of separated NT aggregates with non-compact structure. The next parts III and IV fitted well by the power law $(C-C_p)^t$reflect two stages of electrical percolation with the thresholds at $C_{NT}^{c1}\approx0.02$ wt% and $C_{NT}^{c2}\approx0.5$ wt% corresponding to NT networks of different densities.

[1]. A.J. Twarowski, A.C. Albrecht. Depletion layer studies in organic films: Low frequency capacitance measurements in polycrystalline tetracene // J.°Chem.°Phys. – 1979. – V.°70. – N.°5. – p.°2255°–°2261.

Intermolecular Interactions and Liquid Crystal Properties of Some Cholesteryl Alkanoates

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Cholesteryl n-alkanoates (ChA, further ChA homologues are designated as nChA, where n is number of carbon atoms in the ethereal radical) are important representatives of cholesteric liquid crystals. However, their still many thermal properties, for example, 1-2 and 7-8ChA have monotropic cholesteric transition, 3-6ChA– enantiotropy, do not find the acceptable explanation.

Results of a research of a molecular structure and intermolecular interactions of the first eight ChA homologues (1-8ChA) by methods of infrared spectroscopy and quantum-chemical calculation are given in the present work. 1ChA IR spectra in the field of 4000-400 cm^{-1} in solid crystalline, cholesteric and isotropic liquid phases, and also in solution in the CCl_4 were measured by UR-20 spectrophotometer. Semi-empirical quantum-chemical calculations 1-8ChA were carried out by the AM1 method in the MOPAC program.

IR spectrums of absorption show that in a solid crystalline state at 295 K molecules 1ChA are united in dimers by means of intermolecular hydrogen bonds. At high temperatures in solid crystalline, liquid crystal and isotropic liquid states of 1ChA there is in the form of dimers, a *trance* - and *cis*-isomers. Equilibrium a dimer – *trans*-isomer – *cis*-isomer with temperature increase is displaced to the right.

Quantum-chemical calculations show energy advantage of formation of dimers, lengthening of C=O bond and low-frequency shift of frequency of C=O stretching vibration in dimers concerning monomers 1-2 and 7-8ChA. For 3-6ChA such changes are not observed.

Thus, it is possible to draw a conclusion that molecules 1-2 and 7-8ChA can be united in dimers by means of intermolecular hydrogen bonds. In 3-6ChA such intermolecular hydrogen bonds are absent.

Formation of intermolecular hydrogen bonds leads to increase in forces of intermolecular interactions, and, as a result, to melting temperature increase. Transition from a solid crystalline state in an isotropic liquid state without formation of a mesomorphic phase when heating crystals 1-2 and 7-8CHA can be explained at once with the fact that their melting points lie above temperature area of existence of a mesomorphic phase.

Numerical Simulation of Reflectance Spectrum of Surface Plasmon Sensor with Liquid Crystal

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The surface plasmon sensor with the layer of the nematic liquid crystal (LC) was theoretically investigated. In the conventional surface plasmon sensor TM-polarized light is incident at the interface between the glass prism and the metal layer. The reflectance spectrum has a dip; its position depends on the refractive index of the investigated medium (analyte). The LC layer was added to the system for electrically controlling sensor. The LC ability to reorient under applied field can improve functional properties of the sensor.

The reflectance spectrum was calculated at different voltages applied to the LC. In contrast to conventional sensor,there is also the dip its position depends on the applied voltage.It can be used for measurements [1] or as a reference similar to the case [2]. By changing the LC orientation one can control the dip position and choose the one that is the most suitable for the case.

[1]. V.Yu. Reshetnyak, I.P. Pinkevych, V.I. Zadorozhnii, D.R. Evans. Liquid Crystal Control of Surface Plasmon Resonance Sensor Based on Nanorods // Mol. Cryst. Liq. Cryst. – 2015. – V. 613. – N. 1. – p. 101 – 120.

[2]. M. Abutoama, I. Abdulhalim. Self-referenced biosensor based on thin dielectric grating combined with thin metal film // Optics Express. – 2015. – V. 23. – N. 22. – p. 28667 – 28682.

Enhancement of Nonlinear Optical Response in Hybrid Liquid Crystal Cells with Photonic Crystals

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One of the priority direction of the fundamental nano-science is the use of different nano- and micro-structured surfaces to enhance physical properties of materials deposited on such surfaces, including optical, electrical and other properties. In our research, we investigate the possibility of strengthening of nonlinear-optical response in liquid crystal (LC) cells which is due to the influence of inhomogeneous structured surfaces of substrate, which form the LC cells. For this purpose, we create hybrid LC cells, which consist of two different substrates: the first substrate is a usual glass one, but the second substrate contains a microstructured surface. In our case that was a Si plate of a photonic crystal in a micrometer range. The hybrid cell is filled by the LC between these two substrates.

The photonic crystal structures have been fabricated by different types of lithographic technique. We detailed investigate the scanning electron microscopic (SEM) and focused ion beam (FIB) images of the obtained photonic crystals with the respect of their connection with the fabrication processes. The nonlinear optical parameters are determined by the dynamic holographic technique. We obtain that the effective third-order nonlinear optical susceptibility is enhancement in the hybrid LC cells with the photonic crystal substrate to compare with the traditional LC cells formed by two flat substrates.

5

Biomolecules and Polymers

Tracking of Amyloid Fibril Formation by Chiral Spectroscopic Methods

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Fibrous protein aggregates, β-amyloids, are implicated in a variety of neurodegenerative disorders such as Alzheimer or Parkinson disease. Understanding of protein folding and misfolding leading to the formation of amyloid fibrils may be important for their better diagnostics and treatment. Traditional techniques for protein structure determination, such as X-ray or NMR, are often not usable to study such protein structures in solutions. A limited solubility and molecular size of β-amyloids leads to many other problems.

In the presented work, vibrational circular dichroism (VCD), circularly polarized luminescence (CPL) and fluorescent spectroscopy were used to study fibrous protein aggregates formed by polyglutamic acid (PGA) and hen egg-white lysozyme (HEWL). VCD proved to be useful in detection of such structures because they often provide an enhanced VCD signal (Fig. 1A), but the measurement takes a long time. CPL of $EuCl_3$ and europium complex of $Na_3[Eu(DPA)_3]$ measured on a Raman optical activity instrument provides such information more quickly (Fig. 1B). Currently, we investigate the possibility of using lanthanide luminescent probes to detect formation of other protein fibrils.

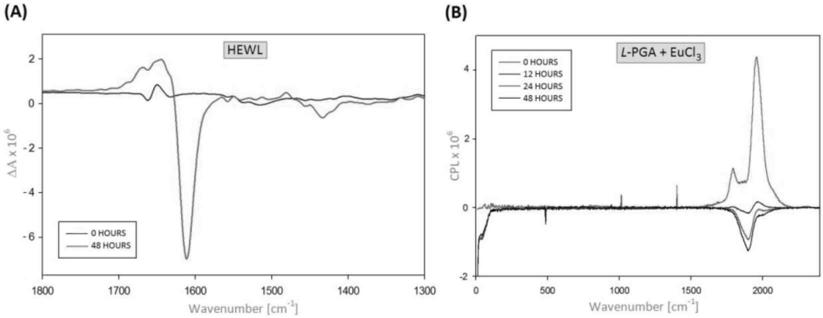

Fig. 1. VCD and CPL spectra of amyloid aggregates.

Manifestation of Optical Vibrations in Thermoluminescence of Organic Polymers

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The release of trapped charge carriers is one of the key processes contributing to the formation of the thermally stimulated thermoluminescence (TSL).In the report the mechanism of such release, which occurs due to absorption by the trap of molecular vibration, is considered. After the irradiation of a sample and producing localized carriers there, the system is brought to a non-equilibrium state. The vibrational subsystem is coming to the equilibrium earlier than the electronic. As a result, the vibrations are in equilibrium, while the charge carriers are still on traps. Energy of vibration quanta is transferred to carriers, releasing the latter from traps. In the work TSL curves, activation energies and Raman spectra of the polymers with varying degrees of ordering: poly(di-n-hexylsilane), poly(methylphenylsilane) and poly(di-n-penthylsilane) were measured and the features on TSL curves were observed. Activation energies of localized charge carriers were found by the fractional thermally stimulated luminescence in the 5 – 50 K temperature range. In order to ensure that the additional features on the TSLcurves are not induced by noise, the measurements were carried out for three substrates: metal, sapphire and quartz.The shape of the TSL curve was calculated taking into account that the release of carriers from traps may be activated via the energy transfer from the vibrations to the carriers. The model explained the coincidence of the carrier’s activation energies with the vibration quanta [1] and the appearance of the features on TSL curves [2, 3]. It is observed experimentally and supported by calculations that the decrease of the degree of the polymer ordering causes the decrease of the numbers of both the discrete values of activation energies and the features on TSL curves.

[1]. Gumenjuk, N. Ostapenko, Yu. Ostapenko, O. Kerita // Low Temp. Phys .- 2012. – **38.** - 932 – 937.
[2]. V.I. Sugakov, N.I. Ostaptenko // Chem. Phys. – 2015.- **456**. - 22 – 27.
[3]. V. Sugakov, N. Ostapenko, Yu.Ostapenko, O. Kerita, V. Strelchuk, O. Kolomys, A. Watanabe // Ukr. J. Phys. – 2016. – **61.** 531 – 536.

Mobile Electronic Excitations in Polynucleotides and Oligonucleotides

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It is known [1-3] that UV-light or penetrative radiation causes mainly the appearance of electronic excitations in synthetic and bio-polymers. Due to weak interaction between pi-electron systems of macromolecules these excitations move along the polymeric chain and finally are captured by some traps. The peculiarities of processes of absorption and migration of this mobile electronic excitations, the nature of traps determine finally the results of radiation-polymer interaction.

This report is the review of the research work on electronic excitation energy transfer (EET) in biopolymers and oligomers as well as on the nature of their fluorescence, delayed fluorescence and phosphorescence [3-5]. The system of first excited singlet and triplet energy levels for DNA and RNA is evaluated using low-temperature (4.2K-77K) luminescent measurements. The traps of the singlet and triplet electronic excitations in these compounds are identified. An important self-protection mechanism against photodamage of DNA and RNA by UV photons or penetrative radiation based on the capture of triplet electronic-energy excitations by the most photostable centers – in DNA, the complex formed by neighboring adenosine (A) and thymidine (T) links; in RNA, the adenosine links – is described. The resulting spreading length of the migrating singlet (l_s) and triplet (l_t) excitations for DNA and RNA macromolecules are evaluated. The spectral manifestation of the telomeres (the important functional system) in DNA macromolecules is examined. The results obtained on telomere fragments provide the possibility of finding the configuration peculiarities of the triplet excitations traps in DNA macromolecules.

[1]. M.Pope, C.E.Swenberg. Electronic Processes in Organic Crystals and Polymers. 2nd ed. – NY: Oxford Uviv. Press, 1999. – 1328 p.

[2]. S.Repetsky, Yu.Onishchuk, V.Yashchuk, Yu.Piryatinski, K.Kushnir, S.Yurchenko // Electron and atomic structure of polymers: Implication for nuclear tracks formation // Radiation Measurements. – 2005. – V. 40. –p. 204 – 212.

[3]. N.Z.Galunov, O.A.Tarasenko. The formation of tracks of ionizing emissions in organic condensed media. – Kharkiv: "ISMA", 2011. – 480 p [in russian].

[4]. V.M.Yashchuk, V.Yu.Kudrya, M.Yu.Losytskyy, I.Ya.Dubey, H.Suga. Electronic Excitation Energy Transfer in DNA. Nature of Triplet Excitations Capturing Centers // Mol. Cryst. Liq. Cryst. – 2007. – V. 467. –p. 311 – 323.

[5]. V.M.Yashchuk, V.Yu.Kudrya. The spectral properties of DNA and RNA macromolecules at low temperatures: fundamental and applied aspects // Methods Appl. Fluoresc. – 2017. – V. 5. – 014001.

Spectral Properties at Low Temperatures of Fluorescent Guanine Substitute as a Probe for Biopolymers Detection

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Deoxyribonucleic acids (DNA) do not show autoluminescence at room temperature and atmospheric pressure. The detection of DNA becomes possible using high-luminescent probes which could be incorporated in the biopolymer macromolecule chain. The best faithful probes of such type are isomorphic nucleoside analogs acting as luminescent substitutes of "native" nucleosides that possess a respectable quantum yield of luminescence at room temperature [1-2]. Herein, the spectral properties of a novel probe – deoxythienoguanosine ($d^{th}G$), a fluorescent substitute of guanine – were studied at room and low temperatures. The optical absorption, fluorescence and phosphorescence (emission and excitation) of $d^{th}G$ were investigated at room temperature and 78K in solution using distilled water and TRIS-HCl buffer.

The positions of the first excited singlet and triplet levels of $d^{th}G$ were estimated and compared with the "native" guanine. Based on this comparison, it is concluded that $d^{th}G$ (if incorporated in the DNA chain) can be the deep trap of singlet and triplet excitations. In $d^{th}G$ solutions, two optical absorption centers that were attributed to two keto-enol tautomers [2], are observed. These tautomers possess additional complete longwave absorption band that is not observed in the "native" guanine correspondent spectra. Both of them are manifested in fluorescence spectra at room temperature in water and buffer solution. At 78K only one emission band is observed in fluorescence spectra. A similar conclusion applies to phosphorescence, as only one phosphorescence band is observed.

[1]. M.Sholokh, R.Sharma, D.Shin, R.Das, O.A.Zaporozhets, Y.Tor, Y.Mely. Conquering 2-Aminopurine’s Deficiencies: Highly Emissive Isomorphic Guanosine Surrogate Faithfully Monitors Guanosine Conformation and Dynamics in DNA // J. Am. Chem. Soc. – 2015. – V. 137. – N. 9. – p. 3185 – 3188.

[2]. M.Sholokh, R.Improta, M.Mori, R.Sharma, C.Kenfack, D.Shin, K.Voltz, R.H.Stote, O.A.Zaporozhets, M.Botta, Y.Tor, Y.Mely. Tautomers of a Fluorescent G Surrogate and Their Distinct Photophysics Provide Sensitive Information Channels // Angew. Chem. Int. Ed.– 2016. – V. 55. –p. 7974 – 7978.

Features Gelatin Triple Helix Formation Under Magnetic Field

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As it's known, the mechanism of formation collagen's triple helix is an important issue, because it's connected with the study of mechanisms of the human body [1]. The solving of the task includes a series of experiments using model systems. To show the mechanisms of formation collagens structures used liquid systems "water - gelatin" [2]. Triple helix formation of gelatin takes place in several stages. On the first stage occurs transition conformation of separate peptide chains of "tangle" in state "helix". And on the second is combining individual helixes in the triple helix.

Kinetics as solitary spiral formation, and further consolidation in the triple associated is connected with the trajectory of movement of individual sections of the peptide chains [1]. In a theoretical paper [1] includes the mechanism of the triple helix, which differs from traditional views. Under this mechanism kinetics triple helix formation depends on the nature of the interaction between single and double helix peptide chain in the final stages of formation of supramolecular structures. The presence of a magnetic field affects the timeline spiral formation in gelatin liquid systems. In addition, the magnetic fields to study the effect of magnetic fields on the actions of the components of the human body according to [3] up to order 1 mT.

The work was experimentally determined the kinetics of forming a triple helix under the influence of a magnetic field, and its absence. The magnetic field increases the rate of formation of the triple helix. It is suggested that the presence of a magnetic field leads to an increase in the speed of rotation of peptide groups and this leads to increased speed of forming a triple helix.

[1]. Collin M. Stultz. The folding mechanism of collagen-like model peptides explored through detailed molecular simulations.// Protein Science, vol. 15, p.2166-2177.

[2]. S. Courty, J. L. Gornall and E. M. Terentjev. Induced helicity in biopolymer networks under stress. // PNAS September 20, 2005 vol. 102 no. 38 p. 13457–13460.

[3]. A. Jandová1, L. Mhamdi, M. Nedbalová and others. Effects of Magnetic Field 0.1 and 0.05 mT on Leukocyte Adherence Inhibition. // Electromagnetic Biology and Medicine, 24: p. 283–292, 2005.

Spectral, Photophysical and Generation Properties of Rhodamine B Laser Dye in Polyurethane Matrices

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Transparent polymer materials are found to have great prospects in the development of optic and laser equipment as matrices for organic dyes due to their availability and low cost. Polyurethanes possess high chemical compatibility with laser dyes; they are one of the few polymer classes, which allow to manipulate their properties in a wide range by changing a ratio of initial compounds, using isocyanate and hydroxyl-containing components of different structures, and also applying various hardening methods.

This work presents results for the investigations of polyurethane matrix effects on spectral and photophysical properties of the Rhodamine B dye from a xanthene class; this dye is a well-studied compound with wide applications in laser techniques. Presence of the carboxyl group in the Rhodamine B molecule assumes possible covalent bonding of the dye with a polyurethane matrix due to its interaction with the isocyanate group –NCO. These interactions between inserted dye molecules and polyurethane polymers can considerably affect spectral characteristics and photostablity properties of the dyes, as we have shown earlier by example of the phenalenone compound [1]. The polyurethane acrylates, hardened by radical polymerization method, and also aliphatic (based on hexamethylene diisocyanate) and aromatic (based on toluene diisocyanate) polyurethanes, synthesized by polycondensation are used in the experiments.

Optical and IR spectroscopy methods allowed to study the effects of polyurethane polymer aliphatic and aromatic components on spectral and photophysical properties of the Rhodamine B dye. Theoretical estimation of Rhodamine B reactive ability to these polymers has been also carried out according to quantum-chemical indexes for the reactive capacity of different isocyanates. Photostability, efficiency and operation lifetime of the laser active elements based on polyurethane matrices have been investigated. The prospects for their applications in the dye lasers have been shown.

[1]. T. Bezrodna, L. Kosyanchuk, M. Stratilat, G. Menzheres, N. Kozak, T. Todosiichuk. Peculiarities of Interactions between 6-Aminophenalenone Dye and Polyurethane Matrix // Journal of Polymer Research. – 2014. – V. 21. – N. 10. – p. 564.

Mutual Effect of Amixin and DMSO in Model Lipid Membrane by the Evidence of DSC and FTIR

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Properties of biological and model lipid membranes are known to be modified by the presence of foreign substances. DMSO is a universal solvent which widely used in biomedical field as cryoprotectant agent and as main or auxiliary substance in different drugs. Its influence on model and biological membranes were studied in a number of works. Amixin (tilorone) is interferon inducer used as antiviral drug with unexplored membranotropic action. It is known that joint drugs membranotropic effect can vary from their individual one. In the present work, we studied individual and combined action of Amixin and DMSO on model lipid membrane of hydrated 1,2-dipalmitoyl-*sn*-glycero-3-phosphocholine (DPPC) by means of differential scanning calorimetry (DSC) and Fourier transform infrared spectroscopy (FTIR).

It was revealed that Amixin and DMSO have the opposite effects on the thermal stability of the gel and ripple phases of the lipid membrane. Thus, Amixin decreases the temperatures of pre- and main transitions in concentration-dependent manner. The joint effect of the Amixin+DMSO was not rigorously additive by concentration. Maximum deviation towards Amixin takes place at 1:1 mass ratio, which could evidence that Amixin has a preference in sorption on DPPC membrane as compared to DMSO. No evidences of the drugs interactions in water medium were revealed by FTIR spectrum.

The effect of the drugs on hydration of DPPC membrane was monitored by antisymmetric stretching mode of phosphate group (1200-1250 cm^{-1}). It known that DMSO decreases DPPC hydration [1]. We found that Amixin has no effect, whereas joint Amixin+DMSO introduction enhances number of H-bounded phosphate groups, i.e. increases hydration of lipid membrane surface.

[1]. M. Ricci, et al. DMSO-induced pertrubation of thermotropic properties of cholesterol-containing DPPC liposomes // Biochimica et Biophysica Acta. – 2016. – V. 1858. – p. 3024 – 3031.

Effect of Hydrogen Peroxide on The Conformational Dynamics of DNA

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Application of oxidative stress and reactive oxygen species for tasks of medicine and in particular oncology is one of the most promising and modern lines of research. It is possible to treat many diseases stimulating the formation of active forms of oxygen by external factors (like nanoparticles, radiation of different frequency range, temperature, etc.). Fundamental knowledge of the mechanisms of influence of reactive oxygen species on important biomolecules such as DNA, can open the way to control these processes. Model experiment on the effects of hydrogen peroxide on the conformational dynamics of DNA was carried out for this purpose.

The sample of high molecular weight DNA of calf thymus (firm “Serva”) and hydrogen peroxide 3% were used in this research.

Study of the effect hydrogen peroxide on the conformational dynamics of DNA was performed by FTIR spectroscopy, because it was the most appropriate for the given conditions. Spectra were registered using IFS- 66 Bruker instrument.

It has been shown that with increasing concentrations of hydrogen peroxide occurs damaging DNA structure, characterized by a gap along the chain (decoupling of bases in certain areas and formation of single chain DNA), oxidation of bases and their modifications. We also observed a change in the structure of DNA, accompanied by the formation of areas of different types of conformations, in addition increasing the alkalinity of the sample is observed.

The Peculiarities of DNA-Ag Nanoparticles Spectral Properties

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The purpose of this work is the study of influence of Ag nanoparticles which are grown on DNA, on the DNA spectral properties.

The results of the optical absorption, fluorescence, phosphorescence in UV and visible spectral range of Ag nanoparticles interacted with DNA are studied. Optical absorption measured at ambient temperature, luminescence spectra obtained at ambient and at 77 K. All investigated materials were in water solution.

It is shown that Ag nanoparticles do not affect DNA absorption spectra at 260 nm, but additionally the separate band near 417 nm is appear.

At the 300 K two fluorescence bands – 350 nm and 525 nm were observed. These bands, in our opinion, can be connected with DNA fluorescence as well as fluorescence of Ag nanoparticles. The nature of these bands is discussed – possibly the band 350 nm can be connected with plasmonic amplification of DNA fluorescence, and the band 525 nm can be attributed to some plasmonic effects on the surface of nanoparticles.

The lowering temperature to 77 K leads to decreasing the fluorescence intensity of DNA, and appearing of high intensity DNA phosphorescence.

Molecular Relaxation Processes in Multiligand Complexes of Serum Albumin Revealed by MD Simulations

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Serum albumin is the most prevalent plasma protein that participates in binding and transportation of great variety of ligands, such as fatty acids, hormones and drugs. Nowadays the protein represents a common model for the *in-silico* drug design. One basic problem in computer simulation of the ligands interaction with serum albumin is the lack of clear picture of the protein mobility mechanisms.

In the present paper, we have applied molecular relaxation spectroscopy to separate the discrete components of manifold dynamics of two multiligand complexes of human serum albumin (HSA). Both complexes comprised six myristic acid molecules and differed from one another by bound single molecule of warfarin. The constant pressure molecular dynamics (MD) simulations of both complexes solvated by water have been performed. The thermodynamic properties of the complexes and the structural properties of the protein have been calculated along the equilibrium segment of MD trajectories. The kinetics of the sample volume relaxation have been monitored after pressure jump. Spectral analysis of the volume relaxation curves revealed seven discrete processes of molecular relaxation with characteristic time constants differing by six orders of magnitude (from 0.5 ps to 0.5 μs). Three slower processes have been related to the local and global conformational changes of the protein, while faster processes have been attributed to various types of mobility of water molecules in bulk solvent and in hydration shell of the protein.

It has been shown that internal protein dynamics is the dominant feature that defines stability of the HSA complexes with both homogeneous and heterogeneous ligands. The regularities of the endogenous ligand influence on the drug binding to plasma protein have been ascertained.

Acknowledgements. We would like to show our gratitude to the Bogolyubov Institute for Theoretical Physics NAS of Ukraine for providing us the access to computer cluster of the Institute during this research.

Transformation of Cytidine and 6-azacytidine FTIR Spectra Under Deuteration

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In this study FTIR spectra of cytidine, 6-azacytidine and their deuterated forms were obtained. These data complement our earlier Raman studies and computational calculations of vibrational modes of investigated compounds [1,2]. FTIR spectra were recorded on Nicolet TM iS50 spectrometer in the range from 680 to 4000 cm^{-1}. Figure below shows FTIR spectra of cytidine (ctd) and deuterated cytidine (dctd) on the left side as well as spectra of 6-azacytidine (6azactd) and deuterated 6-azacytidine (d6azactd) on the right side. Comparison of obtained spectra demonstrates spectroscopic features of deuteration of nucleosides. Some of vibrational peaks in the range from 680 to 1700 cm^{-1} are shifted both to low- and high frequency side

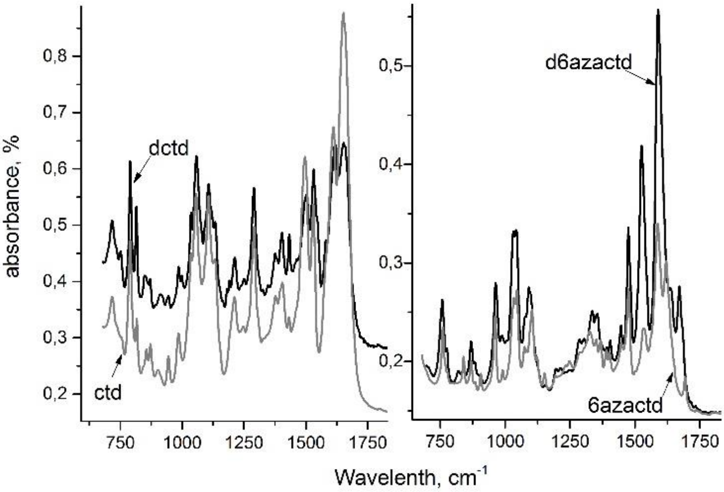

Fig. 1. FTIR spectra of cytidine (left) and 6-azacytidine (right) and their deuterated forms respectively.

[1]. S. Garasevych, M. Iakhnenko, O. Slobodyanyuk and I. Vaskivskyi. Abnormal shifts in Raman spectra of deuterated cytidine and 6-azacytidine// Spectroscopy. – 2010. –24(3-4). – p. 191 – 195.

[2]. S. Garasevych, M. Iakhnenko, O. Slobodyanyuk and I. Vaskivskyi. Transformation of Raman spectra of 6-azacytidine and related compounds// AIP Conference Proceedings. – 2010. – 1267. – p. 664 – 665.

Membranotropic Action of Ibuprofen in DPPC and DPPC/Cholesterol Model Membranes

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Membranotropic action of nonsteroidal anti-inflammatory substance Ibuprofen was studied in model lipid membrane of hydrated 1,2 dipalmitoyl sn-glycero-3-phosphocholine (DPPC) with and without cholesterol. By means of the time-resolved fluorescence anisotropy decay the values of rotation correlation times (φ) and limiting anisotropy ($r\infty$) of perylene probe were obtained in approximation of restricted rotation of anisotropic rotor. This allows estimating the effects of Ibuprofen on microviscosity and ordering of DPPC and DPPC/cholesterol membranes in different phases.

It was found that Ibuprofen impact on membrane microviscosity essentially depends on the phase state of the lipid membranes. It has fluidizing effect (decreases microviscosity) in DPPC membranes in the gel phase and in DPPC/cholesterol membrane in both gel and liquid-crystal phases. But it effect was insignificant for DPPC membrane in the liquid-crystal phase. Ibuprofen decreases the ordering of the lipid hydrophobic chains for DPPC and DPPC/cholesterol membranes in both phases.

Spectroscopic Studies of Viral Nucleic Acids

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Mosquito iridescent virus *Aedes flavescens* (AfIV) is a large icosahedral lipid-containing virus which affects mosquitos and freshwater fish. The AfIV virion consists of a core of genetic material (double-stranded viral DNA), surrounded by a capsid (icosahedral protein shell) which is covered by external lipid shell and internal lipid membrane. Infectious pancreatic necrosis virus (IPNV) is a small virus that causes severe disease of salmonid fish. The IPNS virion consists of a double-stranded viral RNA, surrounded by a protein capsid.

The aim of the work was to compare spectral properties of viral nucleic acids – double-stranded AfIV DNA and IPNV RNA – in order to reveal the correlation between different types of nucleic acids and their spectral properties. Such a correlation might be a tool for distinguishing viruses of different type by means of optical spectroscopy.

Measured are room-temperature absorption (UV) and low-temperature ($T = 78$ K) fluorescence, fluorescence excitation, phosphorescence and phosphorescence excitation spectra of the abovementioned nucleic acids.

It is found that fluorescence spectra of DNA and RNA are different whereas phosphorescence spectra have similar structure.

Spectral Properties of Single-Stranded Viral DNA Fragment

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Deoxyribonucleic acids (DNA) are the most important molecules of living cells and DNA viruses. Moreover, DNA fragments are used as antiviral and antitumor drugs. The knowledge of the electronic processes in these macromolecules (especially the behavior of singlet and triplet electronic excitations) can lead to numerous applications, including the development of new effective drugs. Herein, the spectral properties of (-)PBS, the DNA form of the minus primer binding site (GTCCCTGTTCGGGCGCCA) of the human immunodeficiency virus genome [1] and its complementary (+)PBS (TGGCGCCCGAACAGGGAC) sequence were studied at low temperatures.

The optical absorption, fluorescence and phosphorescence of (-)PBS and (+)PBS oligonucleotides were investigated at 78 K. The optical absorption spectra of (-)PBS and (+)PBSdiffers from the correspondent spectra of the equimolar sums of nucleotides that are in their composition. The difference between them at 295 nm is connected possibly with the existence of some stable complex between bases. The fluorescence spectra bands of (-)PBS and (+)PBS are close to each other and to the band of oligonucleotide investigated by us in [2]. The (-)PBS and (+)PBS bands are connected possiblywith the fluorescence of some complexes that are manifested in absorption.The phosphorescence spectra bands of (-)PBS and (+)PBS are close to each other and to the band of dAMP (in the wavelength range 370-470 nm). The difference between (-)PBS and (+)PBS and dAMP phosphorescence spectra (at 530 nm) is connected with an unknown center. Thus, the main centers of triplet excitation capturing in (-)PBS and (+)PBS are A-bases and centers of unknown nature.

[1]. M.Sholokh, R.Sharma, D.Shin, R.Das, O.A.Zaporozhets, Y.Tor, Y.Mely. Conquering 2-Aminopurine's Deficiencies: Highly Emissive Isomorphic Guanosine Surrogate Faithfully Monitors Guanosine Conformation and Dynamics in DNA // J. Am. Chem. Soc. – 2015. – V. 137. – N. 9. – p. 3185 – 3188.

[2]. V.M.Yashchuk, V.Yu.Kudrya, I.Ya.Dubey, K.I.Kovalyuk, O.I.Batsmanova, V.I.Mel'nik, G.V.Klishevich. Luminescence of telomeric fragments of DNA macromolecule // Mol. Cryst. Liq. Cryst.– 2016. – V. 639. –p. 1 – 9.

Peculiarities of Telomere Fragment Spectral Properties at Low Temperatures and Different Preparation Conditions

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The telomere is the end part of chromosomalDNA that contains a large number of repeated sequences of 6 nucleotides TTAGGG and is responsible for the protection of chromosomes. The shorteningof telomeres can lead to apoptosis. In cancer cells, in contrast to normal ones, telomeric DNA is not shortened upon cell division due to high activity of the telomerase enzyme synthesizing the telomeres.Taking that fact into account the methods of the study of telomeric DNA structure have to be developed.It was shown by us [1,2] that the structural changes in telomeric DNAcould be studied by optics spectroscopy.In the present work, the spectral properties of telomere fragment –d(AGGGTTAGGGTTAGGGTTAGGG) (Tel22) under different conditions of sample preparation were investigated at low temperatures.

The optical absorption, fluorescence and phosphorescence of two types ofTel22 oligonucleotide samples (1 –Tel22 folded intoG-quadruplex structure and immediately frozen, 2 – sample 1 heated to 365 K and then shock frozen) were investigated at 78 K.The optical absorption spectra of both samples differ from that of the sum of nucleotides present inTel22. The difference at 295nm is due to the existence of G-complexes present in quadruplex structure [1].Similar differences were observed in the fluorescence of both samples: only the band associated with the fluorescence of G-complexes was observed.The phosphorescence of both samples (in excitation wavelength range 260-300 nm) isthe emission of the complex formed by adenine (A) and thymine (T) chromophores [1,2]. Besides, it was observed the additional structured band in sample-2 phosphorescence spectra (in excitation wavelength range 310-320 nm) that was close to guanine phosphorescence spectrum band. To our opinion, this band can be explained bythe emission of some intermediates formedupon thermal defolding of G-quadruplex structure.

[1]. V.M.Yashchuk, V.Yu.Kudrya, I.Ya.Dubey, K.I.Kovalyuk, O.I.Batsmanova, V.I.Mel’nik, G.V.Klishevich. Luminescence of telomeric fragments of DNA macromolecule // Mol. Cryst. Liq. Cryst. – 2016. – V. 639. –p. 1 – 9.

[2]. V.M.Yashchuk, V.Yu.Kudrya. The spectral properties of DNA and RNA macromolecules at low temperatures: fundamental and applied aspects // Methods Appl. Fluoresc. – 2017. – V. 5. – 014001.

The Study of Effect of *Closo*-borate on Fibril Formation of Insulin

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Amyloid fibrils are filamentous β-pleated aggregates of proteins, their formation is typical to a large group of diseases, e.g. neurodegenerative. Such aggregates are also investigated as basis for functional biomaterials due to their elasticity and assembly ease. Thus, there is an interest in search of molecules that could affect (inhibit or promote) fibril formation. *Closo*-borates are stable, low-toxic, spherical boron clusters that are known as effective agents for boron neutron capture therapy. Here we explored the impact of dianionic *closo*-borate $[B_{12}H_{12}]^{2-}$ on fibril formation of amyloidogenic protein insulin by circular dichroism (CD), fluorescent spectroscopy and transmission electron microscopy (TEM).

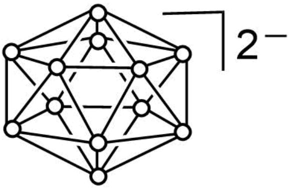

Fig. 1. $[B_{12}H_{12}]^{2-}$ structure

CD studies of $[B_{12}H_{12}]^{2-}$ impact on fibrillization reaction reveal that cluster presence leads to faster transition of insulin from α-helix (bands at 208, 222 nm) to β-sheet (band at 218-220 nm) structure compared with free protein. Besides, the higher content of irregular regions in insulin intermediates induced by *closo*-borate presence was shown. Monitoring of aggregation kinetics by fluorescent amyloid-sensitive cyanine dye shows earlier and more pronounced signal appearance upon fibrillization pathway in boron cluster presence compared with free insulin. This could be connected with the formation of prefibrillar intermediates having β-pleated structure that is induced by$[B_{12}H_{12}]^{2-}$. TEM data point out fibrils formation in both *closo*-borate absence and presence. Free insulin forms branched species (~13 nm in diameter), the fibrils induced by $[B_{12}H_{12}]^{2-}$ have bigger diameter and higher tendency to lateral sticking into large aggregate clots. It is supposed that *closo*-borate effectively binds partially unfolded aggregation intermediates and hence affects kinetic of insulin fibril formation and fibrils morphology.

We express our appreciation for TEM studies conducting to Center for Shared Use of D. Zabolotny Institute of Microbiology and Virology, NASU.

Influence of Temperature on the FTIR Spectra of Microcrystalline Cellulose

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Usually the FTIR spectra of complex molecular systems are studied at room temperature (r.t.). The molecular structure as well as some peculiarities of intermolecular interactions could be determined from these spectra. Variations of temperature, pressure, etc. resulted in phase and structural transitions in studied molecular systems. The FTIR spectra could give additional information on the molecular mechanisms of these processes.In our previous works, we also studied FTIR spectra in wide temperature range and applied models of temperature influence on the spectra, developed by G.O. Puchkovska, for characterization of molecular transitions in similar systems.

The aim of the present work is the study of temperature impact on the FTIR spectra of microcrystalline cellulose (MCC) in the vicinity of relaxation transitions in it. The cellulose is a natural polymer and a basis for a wide range of industrial materials. Among structural modifications of the cellulose, the MCC has a great significance. Temperature-initiated relaxation transition at -100 - 0°C is well-known for the MCC. According to literature data it is related to defrosting of molecular mobility of hydroxymethyl groups, hydroxyls and local motions of the MCC chain segments through the glycoside bonds.The transmittance FTIR spectra of the MCC in KBr pellets were recorded in -150 - 130°C temperature range within 5°C step. Theoreticalanalysisofthetemperature shift of inter-molecular vibrational bands demonstrates that the band shift due to thermal expansion has linear dependence on the temperature.To detect the conformational motion of hydroxymethyl groups, MCC chain segments through the glycoside bonds or primary hydroxyls, the bands at 2930 and 2853 cm^{-1}(asymmetric and symmetric CH_2 stretches of CH_2OH groups), 895 cm^{-1}(glycoside bonds between glucose rings in the MCC chains) and 670 cm^{-1}(C-OHout-of-planebending)were studied in detail.Temperature dependencies of methylene groups stretches have two linear sections (thermal expansion) and a sharp change, corresponding to conformational motion of hydroxymethyl group. At the same time, the wavenumbers of glycoside bands and C-OHout-of-planebending decrease with temperature linearly due thermal expansion, while the conformation transition has no influence on these bands.

Sensitization of Photothermoplastic Holograpic Recording Media with New Cooligomers

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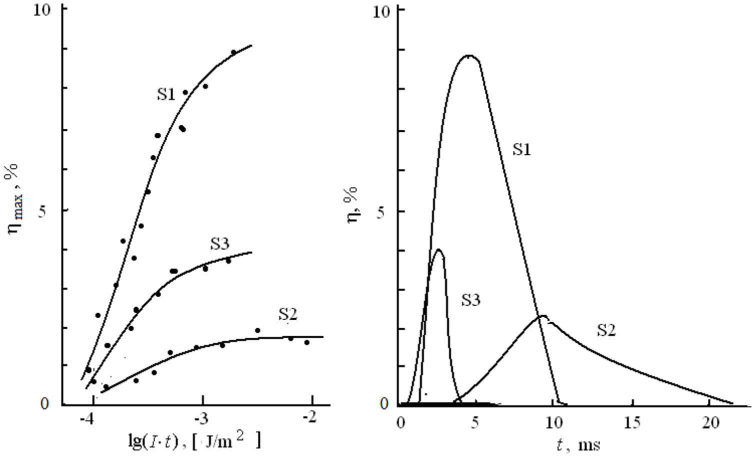
New cooligomers naphthyl-containing oxetane monomers with fluorenyl- (S1), carbazolyl- (S2) and anthracenyloxetane (S3) comonomers were synthesized. Holographic recording media (HRM) based on these cooligomers were developed for the thermoplastic recording technique. 3 mas.% of the compound with intramolecular charge transfer (CICT) was used for sensitization of photoconductivity of the films of the photothermoplastic layer of these HRM. CICT absorption maximum is close to 650 nm allowing to use laser with the same irradiation wavelength. The information properties of the developed HRM were compared.



Dependencies of the diffraction efficiency η_{max} of the holograms of flat wave front on the exposure energy $I{\cdot}t$ and kinetics of development and erasing of the holograms on time t of the recording media heating. Growth ηin the HRM series based on S2, S3, S1 correlates with the changes of T_{soft} and depends on the structure of lateral donor groups of the cooligomer molecule.

Information Characteristics of Cooligomer Holographic Recording Media Doped with Organic Electron Acceptor

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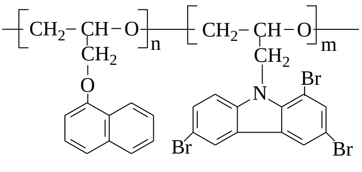
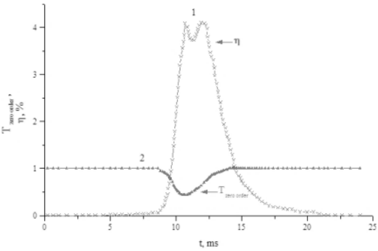
The novel photothermoplastic film holographic recording media (HRM) based on photoconductive cooligomers (Coo1-3) doped with organic dye with intramolecular charge transfer (ICTC) have been obtained. Their spectral, photoconductive, and information properties have been investigated. In prepared HRM, we managed to record holograms of a flat wavefront (HFW) by photothermoplastic method of holograms recording (λ = 650 nm, I = 3 mW, the spatial frequency of hologram recording was $\omega \sim 400$ mm^{-1}. Holograms were recorded at a 1 : 1 intensity ratio of the reference to the object beam).

It was found, that studied HRM films exhibit anomalous polymodal character of the diffraction efficiency change kinetics in the HFW development-erasure process. The features of information properties, as well as the nature of observed effect in the obtained HRM are discussed.



Coo1-3 (n:m = 1:1, 1:2, 2:1)



It was established, that unusual kinetic behavior character of the optical holographic response (diffraction efficiency value з change kinetics) in the hologram development-erasure cycle is associated with a competition between the regular (holographic grating) and irregular ("frost") surface geometric relief formation processes during visualization of a latent image in investigated recording media. Figure shows kinetics of development and erasure of a HFW (diffraction efficiency з value change kinetics) (1), as well as the irregular frost deformation development-erasure kinetics (2) (the frost deformation value ~ excessive light scattering in the HRM ~ $1/T_{\text{zero order}}$, where $T_{\text{zero order}}$ is optical transmittance value in zero diffraction order) in recording medium film based on Coo(1) + 3 mass. % ICTC.

Structural Features of DNA Under an Influence of High-Energy Ionizing Radiation

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A molecule of deoxyribonucleic acid (DNA) is a unique structure, since it is present in a cell in one copy and no other molecule to be able to replace its functions. DNA can be considered as a macromolecular target for the action of radiation and its damage is the most fatal consequences for cell.

Despite of it ionizing radiation influence on biomolecules remains actual topics and important for application, especially in - protectors search. In this work, we propose to consider the ionic solution based on DNA molecules as a model of natural protector against radiation.

Irradiation by electrons with energy 1 MeV of aqueous solution of DNA and buffer DNA solution by different doses was done with linear electron accelerator “Argus” at room temperature. The infrared spectra of experimental samples were registered with a Fourier spectrometer IFS-66 Bruker. In this work, we compared spectrum of reference DNA, in an aqueous and buffer solution with those for DNA irradiated with different doses from 10 to 100 kGr. As a result of analysis, we got that effects of ionizing radiation on aqueous solution of DNA leads to the destruction of the secondary structure for small doses 10-40 kGr. In the case of bigger doses (40-100 kGr) it leads to damage of secondary and primary structure, breaks and formation of low molecular fragments.

DNA in buffer ionic solution is underwent less damage in comparison with DNA in aqueous solution. Thus, buffer solution containing ions can be protector of DNA in the cell. Thus, DNA components in ionic environmental could be proposed for development of ionizing radiation protector.

Donor/Acceptor Properties of Purine and Pyrimidine Bases

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The results of numerous studies show that many properties of NA bases,adenine (A), guanine (G), cytosine (C), thymine (T) and uracil(U),depend on relative positions of their frontier molecular levels. The MO energies can be estimated experimentally [1] or quantum-chemically [2]. It was earlier proposed todefine the donor/acceptor properties of the conjugated molecules by the parameter φ_0 connecting with relative positions of the frontier levels: φ_0 =(ε[LUMO]-α)/(ε[LUMO]-ε[HOMO]), where α is an energy gap middle of reference molecule, for example, polyene with balanced donor and acceptor abilities. Similar approach was used for theoretical estimation of the donor/acceptor properties of NA-bases, when φ_0= 0.5. The calculations gives φ_0< 0.5 for high acceptor pyrimidine bases and φ_0> 0.5 for purines with their prevalent donor property (Fig.**a**). The donor/acceptor parameter is shown to be experimentally estimated by electron affinities [2], ε[LUMO], and electron transition energy, (ε[LUMO] - ε[HOMO], (Fig.**b**).

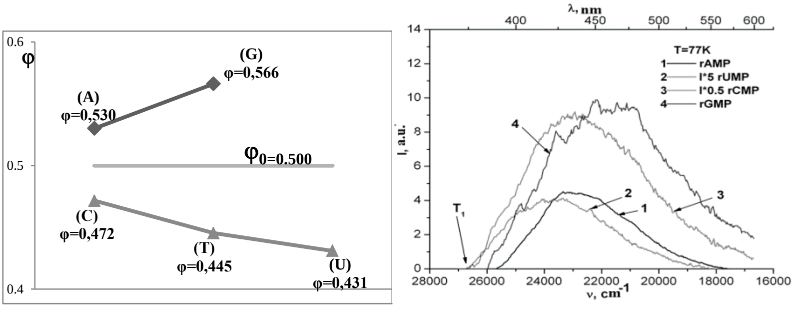

Fig. 1.The donor/acceptor parameter φ for purine and pyrimidine bases ***(a)*** and phosphorescence spectrum ribonucleotides ***(b)***:the aqueous solution; excitation wavelength λ_{ex}=260 nm, $C_{rAMP,rCMP,rGMP,rUMP}$=0.34 mM.

[1]. V.A. Ovchinnikov, D. Sundholm. Coupled-cluster andden sity function altheorystudiesoftheelectronic 0–0 transitionsofthe DNA bases. //Phys.Chem.Chem.Phys.– 2014. –Vol. 16. – p. 6931 – 6941.

[2]. D. Svozil1, P. Jungwirth, Zdeněk Havlas. Electron binding to nucleic acid bases. Experimental and theoretical studies. //Review. Collect. Czech. Chem. Commun. – 2004. – Vol. 69.–p. 1395-1428.

Elastic Anisotropy of Hydrogels and Automated System “KERN-DP”

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The ionization of hydrogels with thickness layers $h = 2 \div 4 * 10^{-3}$ m was carried out by the relativistic electrons irradiation with energy of $W \approx 1$ MeV. The dependences of efficiency of the radiation cross-linked were investigated after mechanical characteristics from the fluence, dose of irradiation [1]. The cross-linked hydrogels (CLHG) hydrophilicity and gas-penetrability were investigated as the function of them chemical composition and terms of electrons irradiation.

The quasilongitudinal USvelocity $V_{\parallel} = 9$ m/sec, elastic module $E = \rho \cdot V_{\parallel}^2 = 82{,}70$ KPa; “fast” quasitransversal US velocity$V_{\perp} = 5$ m/sec, shear module $G = \rho \cdot V_{\perp}^2 = 25{,}53$ KPa of radiation CLHG + 10% $(C_2H_4O)_n$ were determined from the oscillogram in Fig. 1.

By means of the automated system “KERN-DP” on programming of Delphi 7 language, which used the program Surfer 10 for the numerical and graphic analysis and the visualization in the automatic regime of these US measurings of anisotropy parameters of elastic waves velocities the Puasson coefficient $\mu = 0{,}2768$ of radiation CLHG + 10% $(C_2H_4O)_n$ was determined.

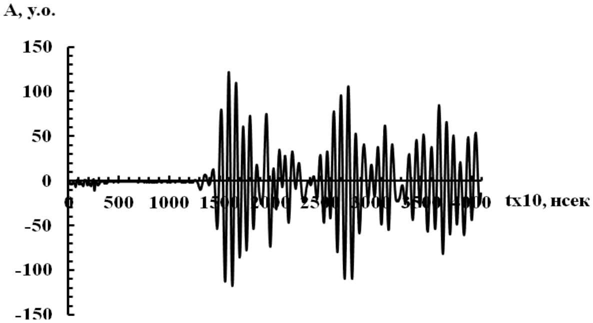

Fig. 1. Oscillogram of impulses with quasitransversal “rapid” polarization $V_{\perp}$in radiation CLHG + 10% $(C_2H_4O)_n$.

The optimum compositions of initial hydrogels and electronic irradiation regimes, which allow to make the radiation cross-linked hydro polymeric composites with the necessary characteristics at the radiation doses $D = 2{,}5 \div 10$ Mrad were founded.

[1] A.P. Onanko, O.V. Lyashenko, S.A. Vyzhva et al. Influence of temperature, ultrasound, electrical current on inelastic-elastic characteristics, relaxation processes in Ge-Si and SiO_2. J. Sensor electronics and microsystem technologies, vol. 2(8), № 3, pp. 14-21, 2011.

Unsymmetrical Relaxation Paths of the Excited States in Polymethine Dyes Detected by Time-Resolved Fluorescence: Polymethinic and Polyenic Forms

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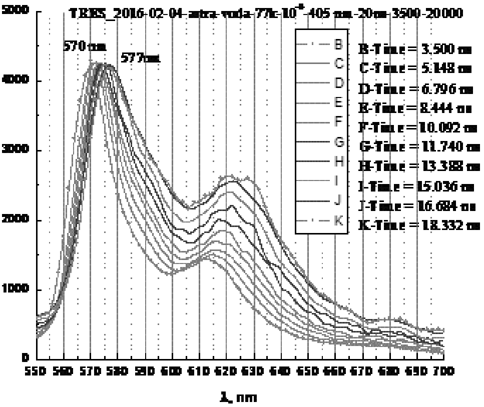
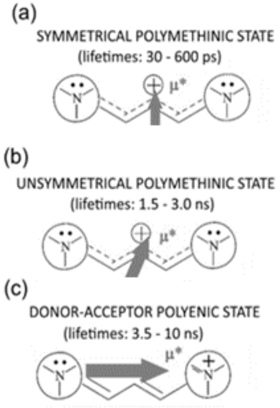
The joint spectral and quantum-chemical investigations of relaxation paths of symmetrical polymetine dyes **1**,**2** and salt **3** are performed. They have shown existence of three relaxation paths:one symmetrical path with a conservation of the symmetry for the electronic structure and two unsymmetrical paths with various symmetry breaking mechanisms. All three components are experimentally detected by time-resolved fluorescent spectroscopy at low temperatures in polar medium (Fig. 1). The fluorescent paths differ by their lifetime and spectral shape (band maxima) as well as strongly depend on rigidity and polarity.





6

Nanoobjects

Computational Studies of Spectroscopic Monitoring of XO_4^{2-} (X = Cr, Mo, W) Oxide Molecular Anions Adsorption on the Surface of Carbon Nanostructures

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Removing of heavy metals from industrial wastewater is an urgent technological need. Carbon nano-structured materials are intensively studied at present as materials for efficient removal and storage of various toxic molecules. The molecular oxyanions are characterized by well-distinguished bands of optical absorption, observed in particular when the anions exist in gaseous phase or are solved in aqueous solutions. The optical absorption bands of XO_4^{2-}anions can be independently predicted in the electronic structure-related computational modeling by calculations of the energies of their excited electronic states and corresponding transition probabilities.

In this work we considered adsorption characteristics of the XO_4^{2-} (X = Cr, Mo, W) molecular oxyanions on the surfaces of pure and N/B-doped CNTs and graphene sheets. DFT-based geometry-optimized calculations of the electronic structures of carbon nanostructures with adsorbed oxyanions were carried out by Gaussian 09 program package [1]. Relaxed geometries, binding energies between the adsorbates and the nanotubes, charge states of the adsorbates, energies of excited states of absorbed XO_4^{2-} anions are calculated and analyzed. The optical absorption spectra of XO_4^{2-} anions adsorbed on the CNTs surfaces are calculated and compared with corresponding experimental data. Effects of water solvent on studied adsorption case are considered with the polarisable continuum model (PCM).

Calculation results are analyzed together with existing experimental data on the optical and luminescence properties of carbon/oxide composites. Possibilities for spectroscopic monitoring of the XO_4^{2-} anions removal from industrial wastes by carbon nano-structured materials are outlined.

[1]. Frisch M.J., Trucks G.W., Schlegel H.B., et al. // Gaussian 09 (Gaussian, Inc., Wallingford, CT, 2009).

The Photoluminescence Nature of $PbCdI_2$ Films

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As we showed earlier [1,2], the prospectivity of $Pb_{1-X}Cd_XI_2$ layered semiconductors lies in the possibility of the developing on their basis of scintillation materials for detecting X- and γ-rays. The intense photo- and radio-luminescence (PL and RL) of these crystals at room temperature is associated with the natural formation of PbI_2 nanoparticles (NP) embedded in CdI_2 matrix during the growth of the solid solution. The presence of such nanoparticles creates a number of new energy levels which are characterized by radiative recombination even at room temperature, and also causes the manifestation of a quantum-size effect for the quasiparticles inherent to these crystals.

The aim of the work is to obtain a film with a large concentration of PbI_2 NP of controlled sizes with optical properties similar to those of bulk crystals. $Pb_{1-X}Cd_XI_2$ films were prepared by drying of solution with molar ratio $PbI_2/CdI_2 = 0.3:0.7$ in absolute N,N-Dimethylformamide (DMF) at 90°C. The investigation of the surface structure of these films using an atomic force microscope showed the presence of nanoparticles with sizes of 10-60 nm.

The PL measurements of the investigated films at room and liquid helium temperatures have shown bands similar to those which are observed for $Pb_{0.3}Cd_{0.7}I_2$ bulk crystals. In the PL spectrum of $Pb_{0.3}Cd_{0.7}I_2$ films at room temperature, an intense wide band with a maximum at $\lambda = 594$ nm appears. In the PL spectrum at $T = 4.2$ K, a narrow emission line of free excitons with a maximum at $\lambda = 495$ nm, a narrow band with a maximum at $\lambda = 508$ nm caused by the recombination of donor-acceptor pairs, an intense band with a maximum at $\lambda = 550$ nm, caused by the recombination of localized excitons on stretched Pb-I bonds on the surface of nanoparticles, as well as the G1 band with a maximum at $\lambda = 594$ nm appear. The nature of these bands was identified on the basis of a deep analysis of the temperature dependence of the investigated crystals photoluminescence, in particular, the temperature dependence of the energy position of the bands, their integrated intensity and half-width [1].

[1]. A.P. Bukivskii, Yu.P. Gnatenko, Yu.P. Piryatinskii, R.V. Gamernyk // Journal of Luminescence. – 2017. – v. 185. – p. 83 – 91.
[2]. A.P. Bukivskii, A.O. Sofiienko, V.Ya. Degoda, R.V. Gamernyk, Yu.P. Gnatenko // Materials Science in Semiconductor Processing – 2017 – V. 67. – p. 28 – 32

Kinetics of Photoluminescence of $PbCdI_2$ Solid Solutions

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Semiconductor $PbCdI_2$ crystals are promising materials for the development of radiation detectors, since they exhibit intense photoluminescence (PL) and luminescence excited by X-rays at room temperature. It should be noted that these materials are promising for the manufacturing of scintillator detectors. The use of $Pb_{1-X}Cd_XI_2$ solid solutions may extend the spectral region of radiation and improve the scintillator properties of existing detectors.

The conducted studies of PL spectra and in-depth analysis of their temperature dependence [1] made it possible to establish the nature of PL bands and to construct an energy diagram of optical transitions in the investigated crystals.

The time-resolved PL studies, carried out in this paper, provided information on both the response speed of the materials and the nature of the emission as well as the dynamics of the electronic processes that cause such photoluminescence.

The PL kinetics of $Pb_{1-X}Cd_XI_2$ crystals (X = 0.7) were measured using the lifetime spectrometer LifeSpec2 at room temperature and 4.2 K at different wavelengths. Analysis of the PL signal decay was carried out by two methods. The first one is based on the fitting of the PL decay using a stretched exponent $I(t) = I_0 \exp\left(-\left(\frac{t}{\tau_{eff}}\right)^{\beta}\right)$, where τ_{eff} is the effective lifetime, and β is the parameter characterizing the disorder of the system. This method provides the rate constant distribution and the ensemble-averaged lifetime.

The second method is based on the approximation of the decay curve by a large number (N = 200) of exponentials. This method allows you to establish the lifetime distribution function and it`s peaks.

We analyze the PL kinetics and obtained lifetimes of bands that correspond to the radiative recombination of excitons localized on stretched bonds on the nanoparticles surface [1] and PL lines caused by the recombination of donor-acceptor pairs and free excitons.

[1]. A.P. Bukivskii, Yu.P. Gnatenko, Yu.P. Piryatinskii, R.V. Gamernyk // Journal of Luminescence. – 2017. – v. 185. – p. 83 – 91.

Influence of theCa^{2+}Impurities on Luminescent Properties of the EuVO$_4$ Sol-Gel Nanoparticles

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It was found recently that structural morphological and spectral properties of the rare earth orthovanadate nanoparticles can be strongly modified with by alkali earth impurities [1-3]. In the present work we study synthesis procedures, structural features, morphological and optical characteristics of the $Eu_{1-x}Ca_xVO_4$($0 \le x, y \le 0.2$)nanoparticles.

Various methods can be applied for synthesis of the orthovanadates nanoparticles, such as solid state, hydrothermal, solution combustion, sol-gel methods, etc.The sol gel synthesis were chosen as the most promising way to perform an excellent homogenization for nanoscale sizes of particles, high reactivity of the compounds and morphology that satisfy enhanced emission intensity.The $Eu_{1-x}Ca_xVO_4$ samples ($0 \le x \le 0.2$) were prepared by aqueous nitrate-citrate sol-gel synthesis route using citric acid (CA) as a complexing agent. Structure of the synthesized samples was characterised by XRD investigation. Formation of the vanadate groups was also confirmed by the IR absorption spectra. Morphology of the particles was studied by SEM. Luminescence spectra were measured at high resolution equipment using DFS-12 and DMR-23 diffraction spectrometers with excitation by diode lasers, nitrogen gas laser, and xenon lamp.Emission of the samples is observed in the 550 – 730 nm spectral range and consists of narrow spectral lines and undoubtedly, they caused by radiation transitions in Eu^{3+} ions. Structure of the emission spectra depends on the excitation wave length, λ_{ex}, and on the concentration of the Ca^{2+} dopant. Excitation spectra of all the synthesized samples are typical for luminescence excitation spectra of un-doped and doped with Eu^{3+} ions LaVO$_4$ compounds. They contain wide band with peak position at about 320 nm and narrow weak peaks around ~ 405 and ~ 475 nm. It was found, that Eu^{3+} ions form two types of emission centers in the samples under study. The assumption was made that I type centers are formed by the Eu^{3+} ions in their regular positions in the crystal lattice, while the II type centers have complex structure and they consists of Eu^{3+} ions, Ca^{2+} cations and oxygen vacancies.

[1]. Qin C., Huang Y., Seo H. (2013) J Am Ceram Soc, 96, 1181–1187.

[2]. Chukova O., Nedilko S.G., Slepets A., Nedilko S.A., VoitenkoT. (2017) Nano Res Let., 12, 340(11).

[3]. Shinde K.N., Singh R., Dhoble S.J. (2014) J. Lumin. 146, 91-96.

Quantum Chemistry Calculations and Determination of the Structure of Nanoclusters

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In present report we address the problem of structure determination of nanoparticles (NPs) consisting of countable number of constituent atoms, *n*, whichare often called nanoclusters (NCs). In the extremely small size range the structures and properties of NCs depend sensitively on *n* and are quite different from NPs larger than a few nm size which are basically nanocrystals as determined by diffraction and other measurements. Experimentally, structure determination of NCs is very difficult task because of so small size that diffraction techniques are not readily applicable on a single NC, in general. A few exceptions are cluster crystals consisting of identical NCs perfectly arranged in 3D lattice. In all other cases the only option is modeling of NC by means of quantum chemistry. We discuss successes and fails of such approach on the example of NCs of II-VI compound semiconductors.

The mass spectrum reveals a series of stable NCs $(AB)_n$ like magic numbers, n = 13, 19, 33, 34, 48 …., which are a quite peculiar compared with known magic number series. Theoretically, the structure originally proposed is a core-cage arrangement in which the cage is basically a polyhedral atomic shell consisting of puckered six-membered rings of alternating -metal-chalcogen- network added by six of four-membered rings. This polyhedral network was first proposed for NCs of $(BN)_n$, and is calculated as particularly stable at n= 12, 16, 28, 36, …… like in magic NCs. This smoothly organized network is in good contrast to another proposed structure of a traditional bulk wurtzite or zinc blende fragment which remains crystalline lattice in the center with many sharp edges on the surface after structure optimization.

The problems discussed in the report include:

- Choice of calculations method and initial guess of atomic arrangement,
- Can computer try all possible structures?
- What difference in energy is meaningful?
- How much can we rely on automatic structure optimization?
- What if different structures have almost equal energies?
- What structure types can be suggested to try for different compounds?
  - Which cluster properties can be reliably predicted to compare with experimentally observed?

Computational Prediction of ZnO Tetrapod Morphology

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One of the hardest tasks of physical sciences is to predict the structure of a crystal from its composition. In this report, we trace the transition from the smallest ZnO clusters to tetrapod-like morphology with the atomic precision [1].

Mass spectrum of the clusters, produced by pulsed laser ablation of zinc peroxide, reveals an enhanced stability of $(ZnO)_{60}$ and $(ZnO)_{168}$ clusters. We propose a model of the nested T_h symmetric ZnO shells, built as Goldberg polyhedra, which explains these particular magic numbers for ZnO clusters. Quantum chemical calculations from the first principles reveal the symmetry reduction of the clusters, most likely caused by Jahn-Teller effect, so $(ZnO)_{168}$ cluster acquires tetrahedral symmetry. We have calculated and compared the binding energies of $(ZnO)_6$ rings, which are the smallest stable structural units of the bulk ZnO wurtzite structure, to the facets of T symmetric $(ZnO)_{168}$ cluster, and thus confirm the tetrahedral symmetry of preferable growth directions for this cluster. The latter is a necessary condition for the tetrapod-like morphology growth. Moreover, the curvature of the symmetry reduced $(ZnO)_{168}$ cluster facets can explain the known experimental fact of existence of some distribution of angles between the legs of ZnO tetrapods (imperfectness of the tetrapods).

[1]. A. Dmytruk, I. Dmitruk, Y. Shynkarenko, R. Belosludov, A. Kasuya. Zinc oxide nested shell magic clusters as tetrapod nuclei // RSC Adv. - 2017. - V. 7. - p. 21933-21942.

Spectroscopic and Structural Characterization of Cu-Doped Y-ZrO_2

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In recent years, Cu-doped Y-stabilized ZrO_2 (Cu-YSZ) nanopowders are intensively developed because of their catalytic, fungicidal and tribological properties. The most study was performed for Cu-YSZ nanopowders prepared by impregnation method. In this work, optical and structural properties of the nanopowders produced by co-precipitation technique were studied by ATR, diffuse reflectance, photoluminescence, EPR, XRD and TEM methods versus calcination temperature (T=500-1000 °C) and Cu content (1 or 8 mol %). It was found that the T_c increase results in two main processes: (i) the non-monotonic shift of XRD peak positions, the non-monotonic change of absorption band peaked at ~270 nm as well as enhancement of absorption band in the 600-900 nm range caused by dispersed and crystalline CuO; (ii) the phase transformation (tetragonal to cubic and both of them to monoclinic). This observation was explained by, at first, Cu in-diffusion in YSZ grains from the surface complexes at T=500-700 °C. After this, for T>700 °C, Cu out-diffusion occurs followed by the formation of crystalline CuO. Besides, an appearance and enhancement of ZrO_2 monoclinic phase occurs due to the replacement of Cu atoms from lattice sites to interstitials that promotes also theformation of the channels for Y out-diffusion via cation vacancies. The analysis of PL spectra of the powdersrevealed two main PL components peaked at about 550 and 640 nm. An annealing at T=500-900 °C results in the slight variation of total PL intensity, while the PL component peaked at 640 nm increases mainly. The treatment at higher temperature (T=900-1000 °C) leads to appearance of specific green emission (peaked at 514 nm) which intensity increases with the increase of monoclinic phase contribution. This band is assigned to radiative transition in Cu_{Zr} taking into account the correlation of its intensity with the intensity of corresponding EPR signal.The phase transformation as well as PL and PL excitation mechanisms will be discussed. The results of this work show the ways for monitoring of Cu distribution in the Cu-YSZ nanopowders.

Optical Centers of Different Types in Zr^{4+}- and Y^{3+}- Doped Ceria Nanocrystals

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CeO_{2-x} nanocrystals (nanoceria) are widely investigated nowadays due to their strong catalytic, oxygen storage, and antioxidant properties determined by high oxygen capacity and easy reduction of Ce^{4+} ions to Ce^{3+} ones. These properties of nanoceria are in turn determined by both concentration and location of oxygen vacancies in ceria lattice which content can be controlled by variation of treatment atmosphere, nanocrystal size and additional doping of nanoceria by di- or trivalent cations.

The influence of isovalent (Zr^{4+}) and nonisovalent (Y^{3+}) impurity ions on the formation of oxygen vacancies in the lattice of cerium dioxide nanocrystals wasinvestigated. It was shown that the content of oxygen vacancies increases significantly at incorporation of both Zr^{4+} and Y^{3+} ions, and oxygen vacancies are involved in the formation of optical centers of two types: Ce^{3+}-$V^{\cdot\cdot}$-Ce^{3+} complexes and F^0 centers. The relationship between optical centers of various types can be controlled by varying both the concentration of impurity ions and the atmosphere of high temperature treatment.

It was shown that while at low concentrations of impurity ions F^0 centers are the dominant type of defects, while at high concentrations Ce^{3+} -$V^{\cdot\cdot}$-Ce^{3+} complexes are main type of optical centers.

Phosphorescence in the Composite Nano-CdS/polyvinyl alcohol

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Light-emitting properties of semiconductor nanoparticles (NPs) attract vigorous interest due to high efficiency and wide tunability of color which makes them promising for applications in the fields of photonics, biosensing, etc. Incorporation of NPs into polymeric matrices adds new functionality to these materials by combining of intrinsic advantages of polymers with size-dependent properties of NPs. In particular, nanocomposite CdS/PVA is the subject of increasing interest. The majority of previous studies were focused on the intrinsic photoluminescence (PL) of CdS NPs while only few papers discussed the participation of the host polymer in the processes of light emission and excitation.

In the present work we study the new-found phosphorescence phenomena in composite and analyze the role of the polymer matrix in the processes of excitation and emission of light of the CdS/PVA nanocomposite as a whole. Colloidal CdS NPs were synthesized in a water solution of PVA as described. Molecules of PVA served as capping agents that restricted the size of NPs during the growth in the solution and served as a solid film-forming matrix used to accommodate light-emitting NPs.

CdS/PVA nanocomposite shows bright PL that is characterized by two wide PL bands in green (~490-510 nm) and red (~650-750 nm) spectral ranges. These bands are usually ascribed to the emission of shallow and deep traps within a NP or on its surface, though the exact origin remains unclear.

At 5K the phosphorescence with multi-exponential decay was observed for CdS/PVA nanocomposite. Note, that the phosphorescence was reliably observed only in the “green” spectral range while emission in the “red” range faded much quicker. The average characteristic decay time of green PL was about 1.7 sec. While stationary PL spectra of CdS/PVA and PVA are very different, the decay times are rather close. The latter suggests that the prolongated emission in composites is related to the excitation transfer from the matrix to NPs.

Metal-Enhanced Fluorescence of Molecular Aggregates

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Well-ordered molecular nanoclusters called J-aggregates attract great attention due to their unique optical properties, distinctly different from those of the individual molecules constituting the aggregate: narrow absorption band, high oscillator strength, giant third-order susceptibility, resonant fluorescence and etc. Such optical properties of J-aggregates are explained by delocalization of electronic excitations over certain molecules on the chain and the Frenkel excitons formation due to the strong interactions between the molecules within the aggregates.

To improve the optical properties of J-aggregates formed in polymeric films one could use the effect of the fluorescence enhancement as a result of fluorophore interaction with a surface plasmon resonance of noble metal nanoparticles. Exciton-plasmon coupling in “J-aggregate – metal nanoparticle” complexes is under great attention due to novel hybrid electronic states appearing. However, a huge amount of works are addressed to absorption spectra changes with main attention to the case of the maximal exciton-plasmon interaction which corresponds to a strong fluorescence quenching.

In the present work, we have reported the 8 times fluorescence enhancement of pseudoisocyanine (PIC) J-aggregate by the interaction with gold nanoparticles in layered polymer films [1]. The important feature of PIC J-aggregates formed in layered polymer film is the exciton self-trapping which has been revealed due to novel red-shifted wide fluorescence band appeared at low temperatures [2]. Surprisingly, exploring the exciton-plasmon interaction in the PIC J-aggregate at low temperature have shown only free exciton fluorescence enhancement while self-trapped exciton emission appeared slowly decreased. So, metal enhancement of J-aggregate fluorescence could be a novel way for overcoming negative influence of the exciton self-trapping on the fluorescence quantum yield of the aggregates. The best of our knowledge, such possibility has never been discussed previously.

[1]. A.V. Sorokin, A.A. Zabolotskii, N.V. Pereverzev, I.I. Bespalova, S.L. Yefimova, Yu.V. Malyukin, A.I. Plekhanov, J. Phys. Chem. C. 119 (2015) 2743.

[2]. A.V. Sorokin, N.V. Pereverzev, I.I. Grankina, S.L. Yefimova, Yu.V. Malyukin, J. Phys. Chem. C. 119 (2015) 27865.

Generation of Reactive Oxygen Species Induced by GdVO4:Eu3+ Nanoparticles – Methylene Blue Complexes under UV Irradiations

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One of the greatest challenges in current radiotherapy is to provide a lethal dose only to a tumor within the tolerance of essential normal tissues. Photodynamic therapy (PDT) of cancer is based on tumor-specific accumulation of a photosensitizer, followed by irradiation with visible light, resulting in cell death and tumor ablation. Activated photosensitizers transfer energy to molecular oxygen, generating reactive oxygen species (ROS). ROS formed upon irradiation, namely singlet oxygen, have a limited lifetime and ability to migrate from the sites of their formation. Thus, they interact with biologic substrates in the sites of photosensitizer localization, which does not lead to damage of normal tissues.

In the present study, we demonstrate generation of ROS upon irradiation of $GdVO_4:Eu^{3+}$ nanoparticles (VNPs) – Methylene Blue (MB) complexes. VNPs were used as an excitation source for photosensitizer MB. Two methods were used to detect ROS. The first method is based on the use of Coumarin as a probe molecules to validate the appearance of hydroxyl radical (•OH). Coumarin react with •OH to form the highly fluorescent intermediates, 7-hydroxycoumarin. Thus, it is possible to estimate the appearance of hydroxyl radicals in solution using a spectrofluorimeter. The second method is based on an analysis of the absorption spectra and detection of diene conjugates formed as a result of lipid oxidation. Lipids can be oxidized by different ROS (superoxide anion ($O_2^{\bullet-}$), hydroxyl radical (•OH), hydrogen peroxide (H_2O_2), singlet oxygen ($^1O_2$), etc.).

Irradiation experiments under UV light (325 nm) during 30 minutes in the presence of $GdVO_4:Eu^{3+}$ nanoparticles – Methylene Blue complexes were shown generation of hydroxyl radical (•OH) due to the presence of VNPs in the complexes (Coumarin method). In addition, generation of singlet oxygen ($^1O_2$) occurs due to the presence of MB in the complexes (the method of diene conjugates). The obtained data show the prospect of using such a complex in PDT.

$GdVO_4:Eu^{3+}$ Nanoparticles as Energy Donors for Methylene Blue in Fluorescence Resonance Energy Transfer Experiments

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Despite the better understanding of tumor biology and improved diagnostic devices observed in last years, cancer remains one of the world’s most devastating diseases being the second leading cause of death. Unfortunately, conventional anti-cancer treatments have many disadvantages including high toxicity, effects on healthy cells, tissues and organs and variety of side effects. Photodynamic therapy (PDT) is an alternative approach to conventional and developed cancer treatment methods and has been clinically used for treatment of certain kinds of cancers, pre-cancer lesions and other diseases. Despite the numerous advantages of PDT approach, this method has the main drawback, small depth of visible and NIR light penetration. One of the possible ways to overcome this drawback is the use the X-ray luminescent (scintillating) nanoparticles as an excitation or “light” source for PDT activation, which has become a hot topic as a new method for cancer treatment.

In the present study, we discuss the possibility for gadolinium orthovanadate nanoparticles doped with europium ions $GdVO_4:Eu^{3+}$ (VNPs) to be used as an excitation source for Methylene Blue (MB) photosensitizer in water solutions and in $CaCO_3$ microparticles. It has been shown that the addition into the water solution even a small amount of MB provokes strong quenching of both $GdVO_4:Eu^{3+}$ luminescence intensity and lifetime. At optimal MB concentration, the FRET efficiency of about 90% has been obtained. Despite the strong quenching of the donor VNPs luminescence, we did not observe FRET-induced emission of the acceptor MB in water solutions. It could be explained by (i) high intersystem crossing quantum yield for MB with a non-radiative deactivation of the triplet level, (ii) small fluorescence quantum yield and (iii) a small amount of MB molecules in the solution bonded to the $GdVO_4:Eu^{3+}$ nanoparticles (about 10%). Encapsulation of both VNPs and MB in $CaCO_3$ microparticles allowed us to observe FRET-induced emission of the acceptor at photo- and X-ray excitation due to an increase of the local concentration of MB near the VNPs surface.

The long lifetime, large Stokes shift, narrow emission and X-ray excited luminescence make $GdVO_4:Eu^{3+}$ nanoparticles prospective as an excitation source for photosensitizer MB in PDT applications.

Photoluminescence of Fullerene C_{60} Thin Film in Plasmon Coupled Au NPs Monolayer – C_{60} Film – Al Film Nanostructure

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The optical properties of plasmon coupled Au NPs monolayer – C_{60} film – Al film nanostructure were studied in dependence of the fullerene film thickness. The mean Au NPs size is 37 nm, Al film thickness is 5 nm and the fullerene film thickness was varied in the range of 10 – 95 nm. The light extinction spectra of the Au NPs monolayer and the PL spectra of C_{60} thin film were measured. Effects of the fullerene spacer thickness influence on plasmonic coupling of Au NPs with Al film were quantitatively analyzed basing on the dependences of the intensity, wavelength and width of SPR extinction peak of Au NPs and the intensity of PL of C_{60} film on the fullerene film thickness.

The red shift, non-monotonic dependences with maxima of the intensity and width of SPR in Au NPs at the decrease of the spacer thickness were observed and considered as the result of thickness dependent plasmon coupling between Au NPs monolayer and Al film. The non-monotonic dependence with minimum of the PL intensity of C_{60} film on its thickness was also observed. It is important that extrema in the thickness dependences of SPR extinction peak intensity and width and fullerene PL intensity occur at the same thickness value of 50 nm that allows to assume the same physical mechanism of such non-monotonic dependences. We assume that such mechanism is the excitation of the propagating SP-polaritons in Al film by the plasmonic near field waves from the Au NPs. The SP-polaritons excitation leads to additional radiative damping of SP oscillations in Au NPs. The increase of radiative damping causes the weakening of the plasmonic field of Au NPs in the gap between the Au NPs monolayer and Al film that leads to decrease of the fullerene PL intensity. As it is known from the literature the spacer thickness at which the most effective excitation of SP-polaritons occurs is 50 nm that is in full accordance with our result. Thus, the observed non-monotonic dependences can be explained as the result of the existence of certain spacer thickness at which the excitation of SP-polaritons is most efficient.

Optical Properties of Au-InP Porous Nanocomposite

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Nanocomposites “porous semiconductors with metal inclusions” and structures based on them seem to be promising for use in optoelectronics, photovoltaics and sencorics etc. due to their optical and electronic properties which are essentially different from the bulk materials, possibility simply tuning their properties and large surface-to-volume ratio. It was shown that deposition of the Au nanoparticles into the pores of semiconductor matrix leads to photosensitivity increase of heterostructures based on them [1]. This work is devoted to the comprehensive study of optical properties of the Au/porous-InP nanocomposite including optical reflectivity, luminescence, ATR, and Raman measurements.

Nanoporous InP layers with different thickness have been prepared from n-type (100) single crystals by anodization in 5% HCl electrolyte in the galvanostatic regime. Gold was incorporated in porous layer in electrochemical cell by two different techniques: from the solution of the Au salt and using spherical Au nanoparticles with SiO_2 shell. As confirmed by the results of the SEM studies porous layers are partially ordered systems ofcylindricalcavitiesorembeddedtetrahedronsdemonstrating a horizontal-plane correlationbetweenneigbouringpores. Depending on the parameters of anodization process the porous layer properties vary in a very wide range: porosity was from 10% to 70%, diameter of pores was in the range 50 - 200 nm and porous layer thickness was 5 - 90 μm. In the case of the small amount of gold in the composite, the cleavage SEM image exhibits that the individual spherical Au particles with a diameter of 10–20 nm are in the inner surface of the pores. With the increase of the deposited gold amount, the pores in the semiconductor are partially filled with metal particles.

In far IR region we observed surface polaritons excitation, which are very sensitive to the essential parameters of porous composite layers such as porosity, symmetry, free carrier concentration, thickness, etc. The gold nanoparticles in the pores leads to an increase of Raman signal in two-phonon band region due to local modes excitation in metal nanoparticles.

Spatially Separated Copper Dendrites for SERS

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Spatially separated Cu dendrites with different morphologies in pores of SiO_2 matrixes on single-crystal silicon substrate have been produced by template synthesis method [1]. Deposition of Cu nanostructures and their structural features have been comprehensive studied, and mechanisms for formation of compact and dendrite-like deposits in the pores of the SiO_2 template on the *n*-type single-crystal silicon substrate have been established. Spatially separated copper dendrites have been used to investigate the efficiency of Raman scattering enhancement using the aqueous solution of the Rhodamine 6G dye. Factors affecting oxidation of copper nanostructures and methods for protecting Cu dendrite surfaces against corrosion and increasing the signal enhancement factor have been discussed.

This work was supported by the Belarusian Foundation for Basic Research (project No. Ф17М-005).

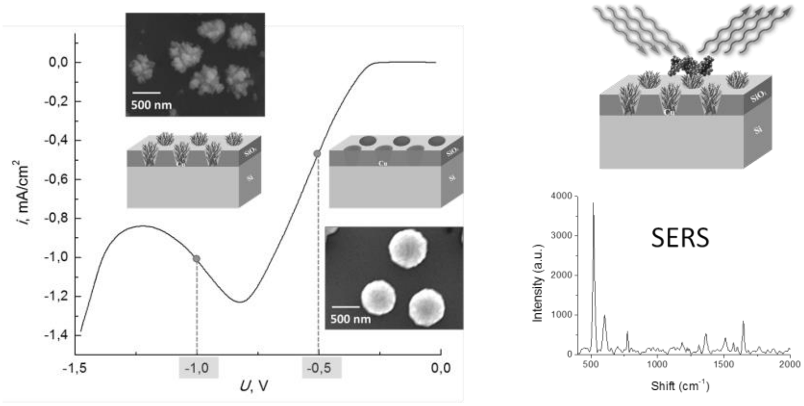

Fig. 1. Control of the shape of Cu nanostructures in pores of SiO_2 matrixes on single-crystal silicon substrate at electrodeposition process and surface enhanced Raman spectrum of the Rhodamine 6G aqueous solution with a concentration of 10^{-6} M on the copper dendritic nanostructures

[1]. E.Y. Kaniukov, J. Ustarroz, D.V. Yakimchuk, et al. Nanoporous Silicon Oxide Templates by Swift Heavy Ion Tracks Technology // Nanotechnology. – 2016. – V. 27. – p. 115305.

Silver Dendrites in Porous SiO_2/Si Template for Single Molecule Detection

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The creation of new efficient and inexpensive plasmon surfaces, which have a large number of plasmon-active areas. It possible to obtain a strong, reproducible and stable signal at Surface-enhanced Raman spectroscopy (SERS) is an urgent task of nanomaterial science. The most suitable structures for SERS are dendrites, which have a lot of “hot spots”. However, using dendrites for detection of single molecules was not carried out because of electromagnetic screening effect and penetration of the analyte under them. In our work, we suggest the solution of this problem by means of spatial separation of silver dendritic nanostructures by template synthesis.

The template was a porous matrix of silicon dioxide on silicon [1] with pores size of 700-800 nm. The formation of spatially separated dendrites in the pores of the template was performed by immersing of SiO_2/Si in the aqueous solution of 0.02 M $AgNO_3$ and 5 M HF for 30 s. Investigation of the enhancement of Raman scattering were carried out on the Ellman's reagent ($C_{14}H_8N_2O_8S_2$) with concentrations in the range of 10^{-4}–10^{-15} M. A green laser with a wavelength of 532 nm and a power of 1 mW within the exposure time of 1 s was used in the experiment. Analysis of the obtained data indicates the possibility of detecting ultra-small concentrations (single molecule) of the Ellman’s reagent, the detection limit of which was 10^{-15} M, and the enhancement factor of the Raman signal reached more than 10 orders of magnitude. Thus, spatially separated dendrites in the pores of the SiO_2 template on silicon are effective plasmon-active surfaces for SERS, which have a record-high sensitivity and can find application in chemo- and biosensorics.

This work was supported by the grant from the Academy of Sciences of Belarus (No. 2017-26-010).

[1]. E.Y. Kaniukov, J. Ustarroz, D.V. Yakimchuk, et al. Tunable Nanoporous Silicon Oxide Templates by Swift Heavy Ion Tracks Technology // Nanotechnology. – 2016. – V. 27. – p. 115305.

Deep Traps in Metamorphic InAs/InGaAs Quantum Dot Structures Studied by Thermally Stimulated Conductivity Spectroscopy

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Levels of electron traps with InAs quantum dots (QDs) grown by molecular beam epitaxy in metamorphic $In_xGa_{1-x}As$ embedding layers with x of 0.15, 0.24, 0.28 and 0.31 on GaAs substrates were studied with lateral thermally stimulated conductivity (TSC) measurements.

The TSC temperature-driven spectra were obtained, illuminating the samples for 30 min at 77 K in the excitation areas from the QD resonant absorption to the GaAs substrate band-to-band generation of carriers (1.6 eV), as well as in the absorption area of defect centers (below the photoluminescence band of QDs), and thereafter were kept in dark for 3 min just before the start of heating from 77 to 300 K.

The spectra show that the samples contain numerous electron traps. Their bands overlap each other, so their location relative to conduction band was roughly estimated considering the maximum of TSC peak position. A set of the traps located at 0.18-0.19, 0.22-0.23, 0.30-0.33, 0.38-0.40, 0.42-0.43 and 0.47-0.48 eV below the conduction band manifest in the TSC spectra of the samples. The sharpest and highest peaks are found on the TSC curves after resonant excitation of the QDs, except the sample with the lowest indium content in the embedding layer. It is concluded that the respective electron traps in the rest of samples are the structure defects near the QDs embedded in the InGaAs matrix.

As for the sample with $x = 0.15$, their TSC peaks are not intense and mostly manifest after the band-to-band excitations within GaAs substrate (1.6 eV) and InGaAs embedding matrix (1.3 eV). This implies that the defect formation due to QD layer growth has been not significant, and those weak peaks on the spectra are mostly related to the defects near InGaAs/GaAs interface.

Magnetic Nanotubes as Carriers for Targeted Drug Delivery

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Nanotechnology allows creating new instruments for biomedicine from diagnostics to therapy [1]. One of them is targeted drug delivery by magnetic field using metallic nanostructures as carriers. The most interesting magnetic nanostructures for biomedical applications are nanotubes, due to their unique characteristics: low density, huge magnetization and predictable behavior under magnetic field [2]. Before they will be used for medical purpose every nanoobject should be comprehensively studied by accurate techniques. Studies of morphological, structural and physical properties as well as *in vivo* and *in vitro* investigations need to be done and an assurance of payloads attaching possibility should be provided.

In this work, electrochemical method of deposition in polyethylene terephthalate templates was used for magnetic nanotubes synthesis. Detailed study of their structural characterization: wall thickness, composition and degree of structural order were carried out by methods of scanning electron microscopy, energy-dispersive and X-ray analysis correspondingly. Magnetic characteristics were studied by mean of vibration magnetometry. Magnetic nanotubes were covered by biocompatible polymer to decrease toxicity and increase adsorption capacity of nanotubes to payloads. Scanning electron microscopy as well as ATR-FTIR-spectroscopy was used to control quality of nanotubes coatings by biocompatible polymer and successful payloads attaching (biological molecule). Moreover, cytotoxicity tests were carried out for coated and uncoated magnetic nanotubes using glioblastoma (the rat glioma cell line C6) and human ependymoma (the cell line E138) cell lines.

[1] K. M. Pondman et al. Magnetic drug delivery with FePd nanowires // J. Magn. Magn. Mater. – 2015. – V. 380. – P. 299–306.

[2] A. L. Kozlovskiy et al. Comprehensive Study of Ni Nanotubes for Bioapplications : From Synthesis to Payloads Attaching // J. of Nanomaterials. – 2017. – V. 2017. – P. 1–9.

Sorption of Polymethine Dyes on Nanographites and Carbon Nanotubes

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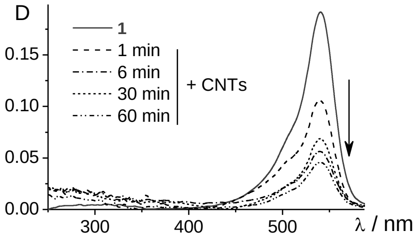
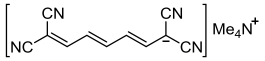
Organic semiconducting functional composites based on carbon nanostructures, such as nanographite (NG) or carbon nanotubes (CNTs), are promising materials for batteries, solar cells, photocapacitors, printed electronics, etc. [1,2]. Highly developed surface of these nanomaterials allows modifying their properties with functional molecules via sorption, eschewing the time- and cost-demanding chemical modification. Polymethine dyes (PDs) are unique photo-energy convertors with the widest known range of photophysical properties variability. Combination of PDs and carbon nanostructures in hybrid composites promises new prospects for their application. Interaction of PDs with carbon nanostructures has been studied in ethanol and aqueous solutions for model cationic (**1**) and anionic (**2**) dyes. With NGs, both bare and modified via oxidation / treatment with diethylamine, the resulting absorption spectra are superposition of the spectral bands of the components, i.e. there is no strong interactions between PDs and NGs in such systems. With single-, double- and multi-walled CNTs, a rapid decrease in dyes' absorption band intensity was observed (Fig. 1) along with the stabilization of the CNT-suspension. Probably, the sorbed dye ions impart CNTs the charge, thereby increasing their solubility in polar solvents and preventing coagulation.





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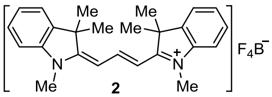

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Fig. 1. UV/Vis spectra of dye **1** in ethanol with double-walled CNTs.

[1]. X. Huang, X. Qi, F. Boey, H. Zhang H. Graphene-based composites // Chem. Soc. Rev. – 2012. – V. 41. – N. 2. – p. 666 – 686.

[2]. M. F. L. De Volder, S. H. Tawfick, R. H. Baughman, A. J. Hart. Carbon Nanotubes: Present and Future Commercial Applications // Science. – 2013. – V. 339. – N. 6119. – p. 535 – 539.

Preparation and Luminescence Properties of Nanocomposite $CaWO_4@SiO_2$

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Nanocrystalline $CaWO_4$ is a promising material for use in X-ray-induced photodynamic therapy (XPDT). This is due to the intense luminescence of $CaWO_4$ and the overlap of its luminescence spectrum with the absorption spectrum of an effective photosensitizer (PS), such as porphyrin [1].

One of the requirements for the realization of excitation energy transfer from the $CaWO_4$ nanoparticle to the PS molecules, which is the main step in XPDT, is the nanoscale distance between the energy donor and the acceptor, which should be several nanometers.

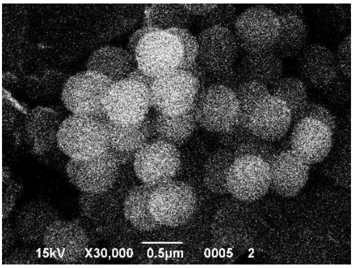

Fig. 1. SEM imagine of nanocomposite $CaWO_4@SiO_2$

The aim of this work was to synthesize the nanocomposite, consisting of a scintillating $CaWO_4$ nanocrystal core and a mesoporous SiO_2 coating, which serves for both PS loading and setting the required distance. The composite was prepared in four steps: (i) synthesis of an amorphous $CaWO_4$, (ii) deposition of a SiO_2 layer, (iii) annealing at high temperature to form a crystalline phase of $CaWO_4$, and (iv) deposition of a mesoporous SiO_2 layer.

According to the SEM and TEM studies, the maid diameter of the nanocomposite was ~ 500 nm. The luminescence spectrum of the synthesized nanocomposite consists of the high intensity broad emission band centered at about 420nm, which is due to electronic transitions of the charge-transfer type between oxygen and tungstate within the anion complex WO_4^{2-} in $CaWO_4$.

Thus, the size and structure of the synthesized nanocomposite will allow us to realize the necessary conditions for energy transfer from the x-ray-induced nanoparticle to the PS.

[1]. H. Homayoni. // Enhancement of protoporphyrin IX performance in aqueous solutions for photodynamic therapy. – 2015. – V. 12. – N. 2. – p. 258 – 266.

Features of Microstructure of Chemically Obtained Graphenelike Particles

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As is known one of the graphenelike structure obtaining methods is chemical treatment of layer carbon materials with strong oxidizers. Such treatment with one hand, leads to the destruction of a lamellar graphite structure and the formation of graphenelike sheets but, on the other hand, stimulates the appearance of a significant number of defects in graphite layers.

The work presents the investigations results of change of nanocarbon particles surface morphology and microstructure after chemical treatment with strong oxidizers and after sonication. The nanocarbon specimens (nanographite particles thickness of (5-10) μm, obtained by mechanical and chemical methods) were treated with strong oxidizers, such as potassium permanganate and organic compounds. Surface morphology and microstructure of nanocarbon particles after chemical treatment were investigated with electron microscopy including high resolution electron microscopy. The EPR method was used for analysis of order degree and defects in graphite layers. Also for determination of the deficiency degree of graphenelike sheets Raman spectroscopy was used.

The presented data reveal that treatment of initial nanographite with strong oxidizer lets get planar graphenelike sheets with length to 50 nm with small number (less than 10) of flawless layers Fig. (1a). The treatment of initial nanographite with less strong oxidizers leds to the formation of ribbonlike highly defective nanocarbon structure Fig. (1b).

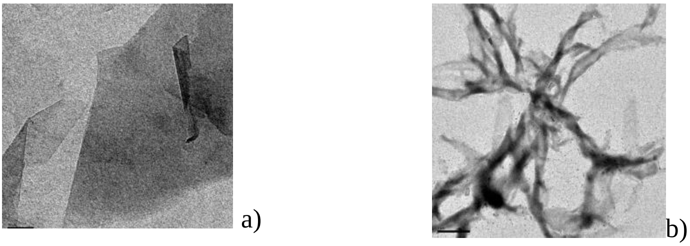
a) b)

Fig. 1. TEM imagines of nanographite plates treated with KMnO4 solution in the sulfuric acid (a) and with acetone (b).

Influence of Dielectric Film Thickness on the Surface Plasmon Resonance in the System “Au NPs Monolayer–Dielectric Spacer–Al Film”

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The purpose of present work was to study the influence of the thickness of dielectric shellac layer on spectral characteristics of SPR in a planar three-layer system: 2D array of Au nanoparticles with a diameter of 90 nm – dielectric shellac film withvariable thickness in the range of 3-200 nm – Al film with thickness of 5 nm, deposited on a glass substrate. The extinction (optical density) spectra of this system were measured. The resulting spectra were peak-fitted by Gauss peak functions. Proceeding from this, we identified the spectral peak of surface plasmon resonance in gold nanoparticles and determined its spectral characteristics such as spectral position of the maximum, total and peak intensities.

It was obtained that decrease of the thickness of shellac caused the considerable (140 nm) red (low-energy) shift of extinction peak of surface plasmons. As well, the non-monotonic dependences of peak and integral intensities of plasmon extinction peak on shellac film thickness were observed. It was obtained that the maximum extinction is observed at film thickness of 70 nm. Another interesting effect is an appearance in the extinction spectrum, besides the low-energy dipole surface plasmon peak, the additional high-energy peak caused by the excitation of quadrupolar surface plasmons, occurring when shellac film thickness is less than 30 nm. As the shellac film thickness decreases, the quadrupolar SPR peak red shifts also, but its shift value is significantly less than one of dipole peak.

The decrease of intensity of dipole peak and synchronous appearance in the extinction spectrum of the quadrupole peak with decreasing shellac film thickness smaller than 70 nm is caused by the hybridization (mixing) of states of dipole and quadrupole surface plasmons. This hybridization is the result of breaking of symmetry of Au nanoparticle surface plasmon field due to presence of Al film. As a result, the probability of optical transitions caused by quadrupolar surface plasmons increases, while the probability of transitions associated with dipole surface plasmons decreases.

Based on the experimental results, we can conclude that the three-layer system “Au nanoparticles – shellac dielectric film – Al film” can be used in nanophotonic devices where there is a need for controllable and smooth tuning of spectral position and intensity of the extinction spectrum.

Infrared Spectroscopic Investigations of Manganese Ferrites

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The manganese ferrites (Fe_3O_4-Mn_3O_4 system) have been under intensive investigations for a long time due to their wide application in microwave ovens and magnetic storage devices, and also as highly active catalysts in producing hydrogen via methane dehydrogenation into ethylene or acetylene.

Manganese ferrites $Fe_{3-x}Mn_xO_4$ (with x from 0 till 1.3) were prepared by employing contact non-thermal plasma technique. All the synthesized samples were composed of regular faceted crystallites with linear sizes from 150 nm to 1600 nm. Reflection spectra of the samples were obtained with using FTIR spectrometer Nicolet iS10. The influence of synthesis conditions (cation ratio and initial pH) on phase composition and crystallite size of manganese ferrites were investigated with employing XRD, DTA, SEM and magnetic measurement techniques.

FTIR spectra over 1200 cm^{-1} are quite independent of the sample composition and due to the presence of water adsorbed on the surface of $Fe_{3-x}Mn_xO_4$micro-granules or embedded into their crystal lattice. The most essential changes in the spectra with changing x in composition occur in the 400 cm^{-1} – 1200 cm^{-1} spectral region, typical to stretching vibrations of Fe(Mn)–O (up to 700 cm^{-1}), Fe(Mn)–OH and Fe(Mn)–OH_2 bonds (over 700 cm^{-1}). These are a red shift (more than 25 cm^{-1}) and a broadening of band, positioned at 715 cm^{-1} in the Fe_3O_4 spectrum ($x = 0$), with raising x up to 0.8. Moreover, new band at 445 cm^{-1} is confidently detected in the spectra of samples with $x = 0.8, 0.9$. Significant spectral redistribution is observed for $x = 0.4$.

According to crystallographic data, metal (Mn, Fe) ions may occupy positions with tetrahedral and octahedral oxygen neighboring. The most probable positions for manganese ions at $x< 1.9$ are tetrahedral positions, corresponding to the Mn^{2+} charge state. The filling of octahedral positions with Mn^{3+} ions starts at $x = 1.0$; their part is no more than 23 % from total quantity of manganese ions, at $x = 1.3$. Thus, the observed changes may be explained by starting the filling of octahedral positions with Mn^{2+} ions. The raising of the 1039 cm^{-1} band in the $x = 0.4$ spectrum may be related to the structural variations in the metal (Mn, Fe) ions neighboring, that results in dipole momentum changing.

DFT Calculation and Raman Mapping and Spectroscopy of Graphene Nanoparticles on the Opal Surface

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Opal based photonic crystals (PC) due to structure periodicity are able to redistribute a spatial electromagnetic field density and concentrate field in the specific local points of opal. It results in an increase of electrical field in the specific opal regions and enhances the interaction between the field and molecules or particles introduced in PC cavities.

Graphene and its composites are widely used in numerous electronic and optic applications, including optical and electrical signal enhancement.

Here we intend to observe an impact of the PC structure on the optical modes of infiltrated graphene particles and possible enhancement of Raman scattering of graphene modes located within opal cavities. Earlier we got 10 times enhancement for DNA molecules placed in the interglobular PC cavities. Raman spectra and field mapping was done by WiTec Alpha 300 RSA+ instrument. For excitation was used 532 nm laser, Si line at 520 cm^{-1} served as wavenumber marker. Software WiTec 2.10.3 was used for spectra registration, analysis and processing. Surface morphology of the samples was studied by the Nanoscope Scanning Probe microscope (Bruker) in taping mode. AFM images were obtained with resolution 125x125 μm^2 and 512x512 pixel. To simulate the electromagnetic field distribution in FC structure, FDTD method was applied. We choose Lumerical FDTD solutions software package to perform the calculation process. Synthetic opal was represented as 10-layer structure composed of 200 nm diameter SiO2 spheres packed in Face Centered Cubic (FCC) lattice.

We registered the main modes of GNP, namely - G, D and 2D modes and got 2.6-3 times enhancement for them for GNP infiltrated in opal in comparison with those for GNP on Si/SiO_2 surface. This data is in good agreement with simulation results performed by FDTD methods. Mapping image of G and D modes at the opal surface and features of RS spectra of GNP in opal are discussed.

Acknowledgement: we thank to FAEMCAR and STCU 6175 projects for financial support

Pulses of Excitonic Condensed Phase in Double Quantum Wells at Steady Pumping: Size Effects

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The study of systems with a large density of excitons is the one of the intensively developing areas in the physics of low-dimensional systems. In particular, the appearance of inhomogeneous spatial structures [1,2] in the distribution of indirect excitons with large lifetime is revealed in laser-irradiated double semiconductor quantum wells, which makes it possible to create their large concentration. In [3], the appearance of structures was interpreted as the formation of a condensed phase due to the interaction between excitons and finite value of an exciton lifetime. In the presence of an external force the exiton structures can move along the crystal in the form of autowaves, similar to the motion of charge fluctuations in the Gunn effect in semiconductors [4]. In [5] we theoretically investigated the possibility of the creation of pulses of the condensed phase as well as controlling their propagation with an external irradiation. The calculations are based on the model of high density excitonic systems. The model is approbated by the explanations of multiple experiments fulfilled for high exciton systems. We predicted the ability to create undamped pulses of the condensed phase in conditions of steady-state illumination and studied their properties and their motion. The setup of the proposed system includes a narrow highly illuminated region and a broad moderately illuminated region that supports the propagation of islands of the condensed phase. Our calculations showed that the pulses appear abruptly as the intensity of the illumination and the value of the external driving force cross certain threshold values. In the report, we studied the parameters of the pulse motion on the size of the illumination region, lifetime of excitons and other parameters of the system. The results show that the sizes of illuminated regions are also critical for generation appearance. If the distance between border of the system and the highly-illuminated region are small, the generation does not occur.

[1]. L.V. Butov, A.C. Gossad, and D.S. Chemla. Macroscopically ordered state in an exciton system // Nature. – 2002. – V. 418. – P. 751– 754.

[2]. V.B. Timofeev. Collective exciton effects in spatially separated electron–hole layers in semiconductors // Physics-Uspekhi. – 2005. – V. 48. – N. 3. – p. 295 – 306.

[3]. V.I. Sugakov. Islands of exciton condensed phases in a two-dimensional system, the distribution of their sizes and coherence in position // Solid State Commun. – 2005. – V. 134. – p. 63 – 67.

[4]. V.I. Sugakov. Ordered structures of exciton condensed phases in the presence of an inhomogeneous potential// Journal of Physics: Condensed Matter. – 2009. – V. 21. – N. 27. – p. 275803.

[5]. V.Mykhaylovsky, V.Sugakov, I.Goliney. Excitation of pulses of excitonic condensed phase at steady pumping // Journal of Nanophotonics. – 2016. – V. 10. – p. 033504.

Investigation of Light Transmittance in Cells with Suspension of Nanoparticles Pigment Red 176 in Electric Field

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In this work, we present results of the optical properties research of suspension of the dye Pigment Red 176 (PR 176) nanoparticles in dodecane by applying an external electric field. Orientation effect of the electric field was investigated by changing suspension dichroism depending on the magnitude of the applied field. The cells were filled with a suspension with the pigment PR 176 concentration in dodecane of 5 and 10 percentages by weight (isotropic phases). The electric field frequency was 10 kHz. In the absence of an external field the particles of the pigment are placed randomly and the sample scatters the incident light. After switching the field on, the particles are oriented along the field direction and the intensity of the light that's passing through the sample increases. After shutting the voltage down pigments nanoparticles returned to their previous state. The field was applied during 0.5 seconds. We obtained dependencies of the intensity of the light that's passing through the cell from the time. Based on this we can say about ultrafast (microseconds) response time. The results of measurements are shown on Fig. 1.

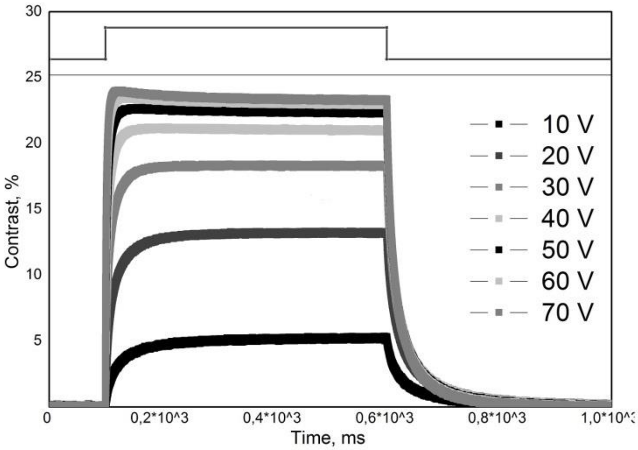

Fig. 1. Dependencies of light intensity on time for different voltages

Application of the Optical Scattering as Remote Method for Characterization of the Surface of Functionalized Carbons

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The present study is directed on the development of an analytical remote optical diagnostics of the surface of functionalized carbons. Typically, nanographite network systems structuring such carbons have open edges, which adopt a nonbonding π-electron state. This edge state exists at the degenerate point between the graphitic π and π^* bands and, definitely, playing a role of the electron reservoir, which is sensitive to the action of the surface functionalization. Respective changes in optoelectronic/magnetic properties of the surface interface can be monitored by optical methods use. To check the hypothesis, an activated carbon fabric (ACF) was used to prepare a series of functionalized carbons, which contain up to 1 mmol/g of bromine. The bromine-functionalized ACFs were studied by elastic optical scattering indicatrix analysis at wavelength 532 nm. The obtained data were interpreted within the data of thermal analysis, and the information obtained by the use of X-ray photoelectron spectroscopy and temperature programmed desorption mass spectrometry. We have found the following correlations between (i) the scattering in the forward hemisphere and the concentration of chemisorbed bromine and (ii) the scattering in the backward hemisphere and the integral intensity of HBr^+ ion current in the mass spectrometry profiles [1]. The proposed technique can be used for the express remote fabrication control of the nanoporous carbons with a given interface.

[1]. Multian et al. Nanoscale Research Letters (2017) 12:146. DOI 10.1186/s11671-017-1873-7

Controlling Light Transmittance of Silver Nanoparticle Ensembles via Surface Plasmon Resonance

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Manipulation of the properties of light and other electromagnetic radiation is a key issue in a large number of practical applications. Among different approaches being used in modern photonics and optoelectronics surface plasmon resonance and related phenomena have become a promising basis of a new type of devices. Recent advance in manufacturing of various structures in micro- and nanometer scale paved the way for a novel scientific and technological discipline named plasmonics. Surface plasmons (SP) are collective oscillations of conducting electrons at the interface between metal or highly doped semiconductor and dielectric surrounding. In the case of nanoparticles surface waves are confined (localized) within the particle’s volume. Since the frequency of such excitations is in resonance with the frequency of incident electromagnetic wave the former termed localized surface plasmon resonance (LSPR). Resonant character of excitations, large curvature of the surface of nanoparticle results in strong enhancement of the local electric and magnetic fields around the nanoparticles. This enhancement triggered a number of applications such as SERS, SEIRA, and nonlinear optics to name a few. In this work, we present some experimental results on manipulation the properties of light passed through Ag nanoparticle ensembles of various types. 2D array of Ag nanoparticles embedded into elastic matrix allows controlling the spectral distribution of transmitted light simply by stretching the polymer film that, in turn, causes changes in distance between nanoparticles. As a result, visual perception of stretched film appear as different colors of the nanocomposite. Those changes can be quantitatively described using color space CIE xyY or CIELAB. Collective plasmon mode originating from coupling of LSPR in adjacent nanoparticles in the array exhibit high sensitivity to the refractive index of surrounding and can be used as corresponding sensor. We also demonstrate the increase of solar cell efficiency by controlling the light scattering patterns with the aid of Au and Ag nanoparticles.

Spectral Ellipsometry of Nanocomposites $(Co_{41}Fe_{39}B_{20})_x(SiO_2)_{100-x}$ with Different Parts of Ferromagnetic Phase

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On the basis of measured ellipsometric parameters Δ and Ψ in the spectral range λ= 0,24-1,0 μm (*h*ν = 1,24-5,15 eV), have been investigated spectral dependencies of optical conductivity σ(*h*ν) of amorphous ferromagnetic alloys in dielectric matrix $(Co_{41}Fe_{39}B_{20})_x(SiO_2)_{100-x}$ for different values of x. Dimensions ferromagnetic particles varied in the range from about 2 to 10 nm. Structural studies of nanocomposites were performed using a scanning atomic force microscope. It was discovered that the optical properties of nanocomposites with different concentrations of metallic phase depend not only on the part of this phase, but also on the properties of the interface areas, and these properties are significantly different at concentrations higher and lower than the percolation threshold.

Luminescent Emission of Undoped and Tb-Doped Cerium Fluoride Nanoparticles in Different Media

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Photodynamic therapy of cancer is based on excitation of the photosensitizer molecule by light; excitation is further transferred to molecular oxygen thus generating singlet oxygen that is toxic for cancer cells. The drawback of this method is the small depth of the light penetration into the living tissue. Thus, the radiodynamic therapy approach was proposed with the X-ray excitation of the sensitizer; the systems composed of scintillating and sensitizing parts with electronic excitation energy transfer (EEET) from the former to the letter one are studied as sensitizers. Recently we have studied the model nanosystem consisting of Tb-doped CeF_3 nanoparticles (NP) and photosensitizer chlorin e_6; it was shown that EEET both from Ce^{3+} and Tb^{3+} ions to chlorin e_6 takes place [1]. Luminescence spectrum of Ce^{3+} ions in CeF_3 NP is known to consist of the bands near 286 and 304 nm corresponding to regular transitions in Ce^{3+} ions $^2D_{3/2}\rightarrow{}^2F_{5/2}$ and $^2D_{3/2}\rightarrow{}^2F_{7/2}$ respectively, as well as of the long-wavelength bands corresponding to perturbed states of Ce^{3+} that are attributed to defects of crystal lattice and surface ions [2]. We have recently shown that EEET from Ce^{3+} to chlorin e_6 is accompanied with the quenching of the long-wavelength emission of Ce^{3+} with maximum near 350 nm. Thus long-wavelength emission of Ce^{3+} is crucial for EEET from CeF_3 NP to photosensitizer.

Here we have studied luminescence emission of undoped (CeF_3) and Tb-doped ($Ce_{0.85}Tb_{0.15}F_3$) NP of cerium fluoride in distilled water and in 50 mM TRIS-HCl buffer (pH 7.2) at the temperature 78 K as well as at the room temperature; fitting of the obtained spectra by Gaussian functions was performed. It was shown that changing distilled water by buffer solution leads to the redistribution in the spectral bands with decreasing the contribution of regular transitions bands and increasing that of the long-wavelength ones pointing that the long-wavelength bands of Ce^{3+} emission are connected with the surface of the NP that is consistent with [1].

[1]. M.Yu. Losytskyy, L.V. Kuzmenko, O.B. Shcherbakov, N.F. Gamaleia, A.I. Marynin, V.M. Yashchuk. Energy Transfer in $Ce_{0.85}Tb_{0.15}F_3$ Nanoparticles-CTAB Shell-Chlorin e_6 System // Nanoscale Research Letters. – 2017. – V.12. – 294.

[2]. D.R. Cooper, K. Kudinov, P. Tyagi, C.K. Hill, S.E. Bradforth, J.L. Nadeau. Photoluminescence of cerium fluoride and cerium-doped lanthanum fluoride nanoparticles and investigation of energy transfer to photosensitizer molecules // Phys. Chem. Chem. Phys. – 2014. – V.16. – P.12441-12453.

Ceftriaxone Molecule Conformational State While Interacting with Copper Nanoparticles with the Protein Components of the Cell Membrane

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Antibiotic resistance - reducing the activity of known antibiotics, due to the gradual adaptability of known microorganisms to these drugs.

In particular, today there is a spread of bacterial resistance to ceftriaxone. Ceftriaxone - cephalosporin antibiotic of the third generation - is an effective antimicrobial drug broad spectrum. Bactericidal action of this tool is due to inhibition of the synthesis of cells walls of Gram-positive and Gram-negative bacteria. The benefits include ceftriaxone favorable safety profile \ and dosing, and relatively low cost. This includes traditional antibiotic regimens infectious processes various locations.

Numerous studies have shown that the use of antibiotics in complexes with metal nanoparticles improves their antimicrobial activity, but the mechanism of this action is not installed. Development of individual medical approach requires deep understanding of the nature, complexity specials

Physically current of the therapeutic effect of a drug sold by its molecular interaction with target proteins that carry out specific functions in the body. This interaction can be direct or caused by external factors, for example, as a result of applying electrostatic potential in the presence of different active molecules and others. Usually the interaction is implemented in a complex chemical composition of an aqueous solution of an organism or cell.

In the first stage, it is important to define the features of molecular structure of each compound, the charge distribution, electronic and vibrational properties of the vacuum that determine its behavior. The feasibility study of the spectral properties, including electronic transitions in the study of optical absorption and photoluminescence, infrared absorption and Raman dictated by the need to conformational electronic identification of these compounds and their behavior. In addition, to establish mechanisms for interaction between drugs and proteins important target of quantum chemical calculations. Study of the interaction of the drug ceftriaxone medical components of the cell membrane of bacteria in the presence of copper nanoparticles.

The nature of electronic transitions of molecules ceftriaxone and model of molecules of amino acids corresponding protein components of biomembranes.

The Comprehensive Investigation of Optical Reflectance, Photoelectric and Electrical Characteristics of the Barrier Structures

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The spectral range of resonance modes excitation depends on the size and shape of particles, their local environment and arrangement, which in turn, are determined by the method of deposition, the substrate reflective index [1] and surface microrelief [2]. Deposition of the metal nanoparticles (Au, Ag) on the semiconductor surface (interface) is known as perspective method for increasing the light absorption in semiconductor due to excitation of surface plasmon (SP) in nanoparticles (NP) or of surface plasmon polaritons (SPP) in their periodical arrays and nanowires [3].

An alternative method of the optical losses reduction and surface recombination velocity decrease is to use metal nanoparticles or periodical array of nanowires for excitation of surface plasmons or evanescent waves-surface plasmon polaritons.Indium tin oxide (ITO) was chosen as an alternative to a metal overlayer because of the possibility for high Schottky barrier formation by optimizing the conditions of ITO film preparation.

Theoretical modelling and experimental investigation of optical, photoelectric and electricalcharacteristics of these structures allowed us to determine physical mechanisms of the photocurrent enhancement effect and its dependence on geometrical parameters of microrelief and nanowires controlled with technological regime.

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[1]. S.Z. Malynych, N.L. Dmitruk, I.E. Moroz.Influence of substrate on the optical properties of non-aggregated silver nanoparticles // Eur. Phys. J. Appl. Phys. – 2013. – V. 64. – N. 2.– p. 20402 – 20407.

[2]. T.R. Barlas, N.L. Dmitruk, N.V. Kotova, O.I. Mayeva, V.R. Romanyuk.Self-assembling of metal nanoparticles on patterned semiconductor surfaces (Au/GaAs) // Superlattices and Microstructures. –2005. – V. 38. – p. 130 – 141.

[3]. N.L.Dmitruk, A.V.Korovin, O.Yu.Borkovskaya, A.M.Dmytruk, I.B.Mamontova, S.V. Mamykin. Plasmonic photovoltaics: self-organized metal nanowires on the solar cell surface/interface //Proc. of 27th European Photovoltaic Solar Energy Conference and Exhibition, Frankfurt, Germany, Frankfurt, Germany. –2012. – p. 408 – 411.

Light Emitting Capped CdS Nanoparticles for Bio-Imaging Applications

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Recent advances of fluorescence detection techniques (improvement of spatial and temporary resolution) promoted the development of fluorescent bio-sensors. The advantage of fluorescence detection is fast signal acquisition and precise spatial localization. The up-to-date bio-imaging techniques are based on nanoparticles (NP). However, at present there are certain challenges in applications. They are: cell autofluorescence that often masks the targeted signals; insufficient photostability of fluorescent tags; necessity to protect NP and biomolecules from undesirable interactions. The latter can lead to degradation of either tag or object, or even both of them. Thus, the important task for future development of nano-bio-sensing is to tune the surface coverage of fluorescent tags in order to optimize detection efficiency and to minimize harmful interactions with biological objects.

Here we report on the synthesis of CdS NP capped with CTAB or MKT and analysis of their applicability for histological studies. It was shown that the colloidal solutions of the above NP, being used for fixed tissues treatment, provide rather intense fluorescence that is sufficient for *in vitro* microscopic studies of tissues morphology. The histological specimens dyed with the synthesized NP are very well preserved for long time (> 5 years of storage).

The studies of the fluorescent tags emission demonstrate strong spectral shifts of wide fluorescence bands when the tags interact with different biomolecules/cells. Therefore, using CTAB-coated NP one can achieve two-color imaging of tissues. The reason is that the eye percepts changing of the fluorescence band positions either as red or green color. Thus, the method proposed is the differential method for cells identification.

The crusial issue for application the NP for characterization live cells (*both in vivo and in vitro*) is bio-compatibility. It was shown that the latter strongly depends on the type of capping molecules. In the present study, we applied the synthesized CTAB- and MKT-coated NP for labeling live erithrocites. It was shown that these tags damage the cells. On the other hand, PVA-capped NP, that were used for the same purposes, did not spoil the biological samples, thus, they can be assumed more promising for labeling live cells.

Spectral Validation of the Diamond-Like Structures in Electro-Discharged Onions and Ball-Milled Graphite

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Carbon onions unite properties of multi-layer fullerenes, nanotubes and graphite. Synthesized by the technology of high intensity electrical discharge treatment (~10^4 current pulses up to 1 MA magnitude) of hydrocarbons (C_6H_6, C_6H_{12}, $C_{12}H_{26}$ at al.) onions possess more complicated structure, having diamond-like nanosized nucleus, then traditional ordered ones, produced at nanodiamond (ND) annealing[1,2]. Their Raman spectra demonstrate the D-band shift at constant laser excitation with λ_L= 514.5, 325 and 257 nm (~60 cm^{-1} at λ_L= 257 nm) and excess increase of D-bands frequencies with subsequent reduction of G-bands ones in UV-region. Extra D_K (1170−1240 cm^{-1}) and G_K (1485−1520 cm^{-1}) components in the Raman spectra correspond to vibrationalstates in the region of big wave vectors **k**,and D_K-band is linked with the diamond structure occurrence. It is corroborate by the enhancement of D-band, its narrowing and shifting from 1347 to 1335 cm with a growth of the sizes and ordering of onions. Simultaneous attenuation of the D_K- and G_K-bands disables linking the D-band with disordered graphite structure. Abnormal enhancement of D_K-band intensity in region of 1065-1160 cm^{-1} have been observed in IR-spectrum of ND, annealed at 1000°C. Very strong decrease of D-bands at λ_L=325 and 257 nm, connected with laser-induced phase transition of ND into graphite shell, is convincing evidence of existence of ND-nucleus in the electro-discharged onions. Decrease of density of carbon at phase transition results in inner self-constriction of ND and growth of the frequency $\boldsymbol{\nu_D}$, what enables estimate inner pressure in onion in 200-250 kbar. Formation of intermediate diamond-like structure (IDLS) at graphite ball-milling is proved by narrowing D- and G-bands on 30-40 % and their enhancement in more then 2 times. A high sensitivity of the IDLS to an impact of a laser irradiation of ~1 mW power is established. A presence of the diamond-like structure in the electro-discharged onions is proved by the analysis of Voronoi polyhedra build on the base of structural data, obtained by the RMC modeling and experimental X-ray diffraction diagrams [3].

[1]. L.Z. Boguslavskii, A.D. Rud’, I.M. Kir’yan, N.S. Nazarova, D.V. Vinnichenko. Surface Engineering and Applied Electrochemistry. – 2015. – V. 51. –Is. 2. – p. 105-110.
[2]. A.D. Rud, N.I. Kuskova, L.I. Ivaschuk, G.M. Zelinskaya, N.M. Biliy. Fullerenes, Nanotubes and Carbon Nanostructures. – 2011. – V. 19. – Is. 1-2. – p. 120-126.
[3]. A.D. Rud, I.M. Kirian, A.M. Lakhnik. http://arxiv.org/abs/1412.1982.

Photoinduced Charge Transfer in Heterogeneous Systems as Driving Force in Photocatalytic Processes

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Photoinduced charge-transfer reactions (PCT) are of the most important types of elementary reactions of electronically excited organic molecules in photochemistry, photobiology, as well as in photocatalytic processes in heterogeneous systems. PET in the excited molecular complex on the solid surface includes the accumulation of light energy and light-induced charge separation. Heterogeneous systems contribute to charge separation in excited bimolecular complexes due to such unique properties as a high surface polarity, rigid orientation of the molecules, the presence of an electron donor and acceptor centers and geometric constraints. This work presents a brief overview of the authors' results on the features of bimolecular electron transfer reaction and exciplex formation between adsorbed pyrene (Py) and *N*,*N*-dimethylaniline (DMA) on the surface of inert silica carrier and photocatalyst TiO_2/SiO_2 examined by fluorescence quenching and transient absorption spectra techniques. The quenching of Py fluorescence by coadsorbed DMA molecules on SiO_2 surface is diffusion controlled (a Langmuir-Hinshelwood type of surface reaction) and gives rise to exciplex formation. Photoreaction of exciplex formation and kinetics of fluorescence quenching of Py by DMA on the surface of TiO_2/SiO_2 proceeds a completely different way than on silica. The addition of DMA as a fluorescence quencher of Py results in an unexpected increase in the intensity of the fluorescence as a result of DMA competitive adsorption on the Py adsorption centers - titanium ions, which are fluorescence quencher also. The intensity of the fluorescence of pyrene monomer is a function of the content of TiO_2, which indicates the effective electron phototransfer from Py * to the active surface. Instant absorption spectra recorded signals of the Py radical-cation and Ti^{3+} . It is shown high photocatalytic effectivity of titania-based nanosystems in the degradation of toxic pollutants as inductrial dyes, antibiotics, toxic transient metals in waste water.

Photoconductivity Relaxation in InGaAs-GaAs Quantum Wire Modulation-Doped Heterostructures

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Optical properties and characteristics of charge carrier's transport in quantum-dimensional heterostructures based on semiconductor III-V materials are widely studied in recent years [1]. Such an interest caused by the possibility of introduction of the quantum dots (QDs), quantum wires (QWRs), quantum wells (QWs) to the active region of novel electronic devices, infrared photodetectors, solar cells and semiconductor lasers [2].

The time dependencies of the carrier relaxation in the modulation-doped InGaAs-GaAs low-dimensional structures with quantum wires have been studied as function of light excitation level. The photoconductivity relaxation follows a stretched exponent with decay constant, which depends on morphology of InGaAs epitaxial layers, energy disorder due to inhomogeneous distribution of size and on presence of deep traps.At low temperatures, T<150 K, multiple trapping-retrapping via 1D states of InGaAs QWRs, sub-bands of 2DEG of modulation doped *n*-GaAs spacers as well as defect states in the GaAs environment is dominant relaxation mechanism.

[1]. C. G. Bailey, D. V. Forbes, R. P. Raffaelle and S. M. Hubbard// Appl. Phys. Lett. –2011.–V. 98.–p. 163105.
[2]. T. Numai. Fundamentals of semiconductor lasers//Spring. Jap.–2015.–V. 93.–p. 89-186.

Nanocellulose as the Main Composite Component of Electromechanical Sensors

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Modern electronics is usually made from materials that can not be biodegradable and sometimes potentially toxic. Production of electronic devices today includes processes that require high vacuum and high temperature. However, the service life of electronics is becoming increasingly shorter. It's create not only technological, but also increasing environmental problems. Cellulose is ubiquitous in everyday life. It is renewable, portable, flexible biopolymer [1]. Thus, the development of nanocellulose (CNC) composite for use for flexible electronic circuits is one of the possible solutions to these problems.

However, theoretical knowledge on the electronic properties of composite structures CNC containing does not exist fully. For expansion of information about electronic properties of composite structures with cellulose (Fig. 1), such as the density of electronic states, width of the bandgap, the charge's state of atoms, we calculated their by the electron density functional methods and first-principles pseudopotential on own program code [2].Table 1 shows the estimated data on bandgapfor Gr/CNC at different distances between the graphene layer and cellulose, that simulates mechanical pressure.

Distance, Å	*Eg, eV/atom*
1,09	0,010
0,97	0,006
0,88	0,015

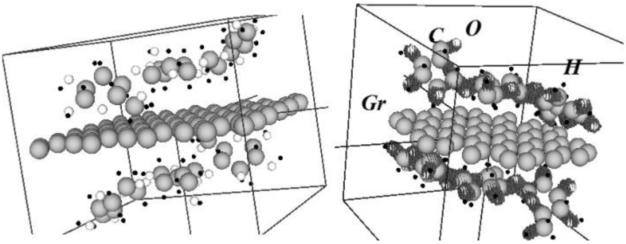

Fig. 1. Hybrid structure based on graphene and cellulose for calculation (left); the spatial distributions of the valence electrons density within the interval of 0.9–0.8 of the maximum value for Gr/CNC

[1]. HORIZON 2020 - Work Programme 2016 – 2017, Cross-cutting activities (Focus Areas), PILOTS-05-2017: Paper-based electronics.

[2]. Ab initio calculation [E-resource] – Mode access to the resource: http://sites.google.com/a/kdpu.edu.ua/calculationphysics.

Energy Spectra Correlation of Vibrational and Electronic Excitations and Their Dispersion in Graphite and Graphene

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Study of the physical nature of the phonon and electron excitations in crystals, especially in high-tech objects promising for planar technologies always has been interesting and important tasks in the physics of condensed matter. This interest caused by the possibility of using of layered structures in micro- and nanoelectronics and the improvement of models of theoretical calculations of electronic-vibrational processes.

Single- and bilayer graphenes as well as graphite via Raman spectroscopy have been investigated. The symmetry of vibrational and electronic excitations for different points of Brillouin zone has been established. The structure and the multiplicity of energy state degeneration have been studied. The graphs of dispersion dependencies and the correlation diagrams for similar points in their Brillouin zones have been built. Compatibility relations of irreducible representations have been established.

For the first time the correlation relations between single-layer, bilayer graphenes and graphite have been established with taking into account the difference in their symmetry groups. These correlations are confirmed by the analytical calculations of the normal vibration forms using matrices of irreducible projective representations.

Effect of Manganese Oxides on Luminescence of Rutile TiO_2

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The couple TiO_2/MnO_x seems to present interesting optical properties, as well as it may be perspective material for solar energy conversion. In the present work, we investigated the luminescence properties of pure rutile (R) TiO_2 powders and synthesized titanium-manganese mixed oxides (TMO) with different Mn content produced by chemical precipitation of manganese hydroxide on pure polycrystalline rutile TiO_2 particles with thermal processing at different temperatures. The morphology, structure and optical properties were investigated by XRD, XRF, EDS, UV-vis absorption andluminescence spectroscopic techniques.

In summary, our research has shown that the optical UV-vis absorption and luminescence properties of nanocrystalline rutile TiO_2 altered with the introduction of titanium-manganese oxides (TMO). XRD analys confirmed the formation of crystalline manganese oxide phases in the form of Mn_2O_3 and $MnTiO_3$. The absorption edge of TMO was found to be significantly shifted to longer wavelengths as compared to pure R TiO_2 that is connected with a decrease in the energy band gap.

Examination of PL spectra excited by the UV laser pulses (at 3.68 eV) revealed the character emission peaks attributed to the luminescence from the surface states localized on the TiO_2 surface (2.4-2.8 eV), to the recombination of free excitons (2.8-3.0 eV) and to the band-to-band transitions (3.0-3.3 eV). The PL quenching for the free exciton emission at 2.92 eV and the near band edge emission at 3.06 eV is connected with the oxygen vacancies in the TMO structure and interpreted by the Auger non-radiative recombination. The relative increase and decrease in the ratio of PL intensities for UV and visible bands with increasing Mn content is due to the concentration quenching effect.

The Synthesis of Silver Nanoparticles in Holographic Photopolymers: Mechanism of Nanoparticle Formation and Their Optical Properties

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Novel materials consisted of noble metal nanoparticles (NPs) embedded in transparent hosts show particularly promising features for the application in modern linear and nonlinear optics, laser physics, and optoelectronics. The micrometer scale structuring of the metal-containing nanocomposites is appropriate for many optical elements such as metal NPs–polymer gratings and photonic crystals. The use of photopolymerizable nanocomposite materials opens the possibility to create sub-micrometer periodic distribution of NPs in polymer matrix by simple one-step method of holographic polymerization.

We present the results of the experimental studies of optical properties of polymer films with random and periodic distribution of silver NPs obtained from composites of different composition. Photopolymerisation of the composite in the interference pattern provide a formation of high-efficient volume grating consisted from the periodicity of polymer and metal precursor-containing regions. A subsequent homogeneous UV irradiation or thermo-treatment of the grating cause the reduction of silver salt to Ag NPs selectively in the areas of the film containing metal precursor. Spectroscopic measurements are reported to confirm the formation of the Ag NPs in the gratings. Transmission electron microscopy showed a regular distribution of well-defined Ag NPs in polymer film with a periodicity governed by the geometry of the holographic structuring.

The physical properties of nanocomposite materials containing metallic NPs in dielectric matrix are determined by the size, shape and spatial arrangement of NPs with micro- or submicrometer scale. The size and the shape of NPs can be controlled by wavelength and intensity of the holographic exposure, by the conditions of post-processing and the composite formulation as well. Possible mechanism for the formation of silver NPs is presented.It was shown that products of photolysis of the used photoinitiating systems are the reducing agents of silver.

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7

Surfaces and Films

Physical and Chemical Properties of Steel Surface Modified by Ionic Implantation

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Modern spectroscopic research methods have acquired great importance in physics and chemistry due to the rapid development of materials science. As a result of applying the achievements of micro and nano materials science, composites and nanostructured materials that are difficult to analyze using traditional X-ray methods were appeared.

In particular, promising ionic technologies, such as ionic implantation, allow the introduction of individual ions and neutral atoms into the surface layer (up to 1 μm) of metals and alloys, thereby creating nanoscale layers. The processed materials have mechanical, physical and chemical characteristics, which exceed several times the original samples.

In the work, samples were synthesized by ionic implantation. Stainless steel was used as initial material. The treatment regime was selected such that the fluence was about 5×10^{17} cm^{-2}.

Studies have shown that synthesized implants have a microhardness of 2-4 times greater than the original steel. The processed steel has a more developed surface - the roughness coefficient is about 3-4. Computer simulation of ionic implantation indicates a small penetration depth of particles (significant concentration at a depth of up to 50 nm). Investigations by X-ray photoelectron spectroscopy showed the presence in the surface layer of implants not only ions of the target material, but also their nitrides, which is due to the presence of nitrogen in the plasma of the ion source.

Thus, despite the low penetration depth of ions, about 100 nm, the effect of ionic implantation is significant. This makes it possible to consider this technology relevant and promising.

Optical Properties of Graphene-Protected Multilayer Structures Based on Noble Metals

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Graphene-protected Ag and Cu is a viable alternative to the conventional noble metals (usually basis on Au) in plasmonics applications. It is relatively cheap, stable, reproducible and high-quality plasmonic material that is suitable for nanofabrication. The HfO_2-protected Cu and Ag provide exciting opportunity for applications which require low plasmonic losses. Such heterostructures as Cr(1.5 nm)/Cu(Ag, Au)(43-47 nm)/HfO_2(7 nm) were prepared. Then two of these structures namely the same Cr-Cu-HfO_2 samples (1) were covered by graphene layer at room temperature and then one of them was annealed at 150°C during 2 minutes (sample 2). Optical properties of all samples were investigated within wide spectral range (photon energy $\hbar\omega = 1 - 4.9$ eV) by spectroellipsometric method based on Beattie-Conn version. The registration of the Fresnel coefficients in p-plane R_p of the film was also fulfilled for an estimation of the level of plasmon excitation effect.

In effective medium approximation, the optical constants as well as dielectric function (optical conductivity σ) of such films were calculated. It seems the optical conductivity spectra of the specimens included thin layer of noble metal (Cu, Ag or Au) clearly remind $\sigma(\hbar\omega)$ dependencies of appropriate pure bulk metal. In the framework of the Drude relationship for these heterostructures the relaxation and the plasmon frequencies were estimated too. The main peculiarity of optical conductivity for sample 1 consists in an appearance of distinct maximum at $\hbar\omega = 1.25$ eV which is slightly widened after sample annealing. Its origin may be connected with interband transitions in surface graphene structure. Plasmonic properties of graphene-protected Cu films were also studied by using the Kretschmann-Raether ATR geometry and distinct minimum was found in their spectral dependences $R_p(\hbar\omega)$. Appropriate plasmon minimum at wavelengths from 580 (at angle of light incidence $\varphi = 53°$) to 680 nm ($\varphi = 47°$) was observed. The covering of glass-Cr(1.5 nm)-Cu(43 nm) structure by graphene essentially (approximately in 4-5 times) widens spectral range where plasmon minimum position is sharply changed. With respect to principal features of optical properties of glass-Cr-Cu-HfO_2 heterostructures covered by just graphene it may be noticed stronger plasmon support for light absorption within range of interband transitions in copper.

Self-Organized Structuring of Surface of Metal-Semiconductor Composite by Femtosecond Laser Processing

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Peculiarities of laser treatment of the composite consisting of thin film of metal (gold) on the surface of semiconductor substrate (silicon (100)) have been studied. Micro- and nanostructuring of the composite sample has been achieved by the irradiation of its initial surface with Ti:sapphire femtosecond laser. The method of direct laser structuring is simple, relatively cheap and allows treating relatively large area of the material by scanning the beam across the sample surface. Controllability and reproducibility of laser structuring process are important for the future applications.

Thickness of the deposited gold film has been determined using Linnik microinterferometer. Surface peculiarities and parameters of obtained laser-induced periodic structures have been analysed by atomic-force and scanning electron microscopy.

Laser structuring of the surface of composite samples requires very accurate selection of laser power density. Under substantial excess of laser power density above structuring threshold sufficient part of energy is released in semiconductor, leading to almost complete removal of gold film. Two modes of treatment of metal-semiconductor composite may have practical value: under slight excess of threshold power (removal of less than half of the area of film) periodic structure is formed at the edges of craters; the second case – under substantial excess of threshold power the metal film is removed and individual metal nanoparticles remain randomly scattered on the rough surface of the semiconductor.

Raman spectra of metal-semiconductor composite are measured under the excitation wavelength of 488 nm. The low frequency shift of 1-3 cm^{-1} of silicon phonon band has been observed for all areas of the sample. This effect indicates formation of silicon nanoislands during the laser processing. Comparing the magnitude of the line shift for the areas with different processing conditions it can be seen certain regularities – the greater intensity of laser radiation, the greater shift of silicon phonon that exhibits the existence of smaller nanoislands. The increase of the band half-width observed for some regions can be explained by the wide size distribution of nanoislands. The band relative intensity decreases for regions with the greatest intensity of treatment that indicates partial amorphization of silicon.

The Study of the Optical Properties of CdTe Thin Films Doped with Ytterbium

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Obtaining CdTe films of high optical quality is a very important task in the physics of semiconductors, since such films can be used to develop on their basis new materials for optoelectronic devices, and for elaboration of solar cells. Incorporation of rare earth elements (RE) into CdTe films leads to the gettering of residual impurities. Thus, their optical quality are improved.

CdTe films doped with ytterbium were deposited by close-spaced vacuum sublimation [1] on a glass substrate under different temperature conditions: the evaporation temperature of CdTe was equal to 700°C and the substrate temperatures T_s = 450, 475, 500°C for different samples, respectively.

It should be noted that characteristic feature of these films is observation of the free exciton in the reflection (ER) spectra at 4.5 K. The free excitons appear at E_{ex} = 1.5964 eV and the distance between the minimum and the maximum of the dispersion curve is about 15 cm^{-1}.

The studies of the photoluminescence spectra (PL) at T = 4.2 K have shown that line at λ = 777.4 nm appears in the exciton region of the PL spectrum due to the recombination of excitons localized on the crystal field fluctuations as well as a line caused by the recombination of the donor-bound excitons (λ = 778.2 nm). In the PL spectrum, the bands (λ = 800.0 nm and 804.0 nm) are also observed due to the optical transitions of electrons from the conduction band to the acceptor level (e-A transitions) and the transitions from the donor level with the ionization energy of 14 meV to the acceptor level. An intense band is observed in the region of 840.0 nm due to the presence of complex intrinsic defects of the acceptor type consisting of a Cd vacancy (V^{2-}_{Cd}) and an ionized donor (D^+). Here in the long-wavelength region the phonon replicas of LO-, 2LO and -3LO are observed.

In addition, in the near infrared region, a band appears whose energy position is E = 1.3137 eV. According to [2], this band can be caused by the intracentral emission of Yb.

[1]. V. Kosyak, A. Opanasyuk, P.M. Bukivskij, Yu. P. Gnatenko, // J. Cryst. Growth 312 (2010) 1726.
[2]. R.Boyn, Phys.Stat. Sol. (b)148 , 11 (1988).

The Photoluminescence Study of CdS Thin Films Doped with Dy

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CdS films with direct band gap energy about 2.42 eV at room temperature have n-type conductivity and high photosensitivity in the visible spectral region. At present, such films are intensively studied mainly because they are suitable material for elaboration of a number of optoelectronic devices such as photo sensors and window layers in the top of tandem high efficiency solar cells based on CdS-CdTe and CdS-Cu(In,Ga)Se_2.

In order to use effectively the semiconductor thin films in micro- and optoelectronics it is necessary to improve their optical, structural and electronic properties.RE elements may be considered as effective gettering agent for residual impurities in semiconductor crystals. In this case RE ions form the complex centers with residual impurities that are electrically inactive. Therefore, doping semiconductor materials with RE atoms allows us to improve their optical quality and electronic properties.

In this work, we study the PL properties of CdSe films deposited on the glass substrates by means of CSVS technique. This let us determine the nature and energy levels of point defects and the presence of dislocations in the films as well as study the effect of growth conditions on their defect structure. As a result of those studies the deposition conditions of CdSe thin films of high optical quality were established.

It was shown that the photoluminescence spectra (PL) of the films obtained at the substrate temperatures T_s equals to 300, 350 and 400 K observe the exciton emission both bound and free excitons at T=4.5 K. Besides, the free excitons are also observed in the low-temperature reflection spectra. In this case, the exciton line is a very narrow that indicates about excellent optical quality of those films. The PL spectra also contain intense emission caused by the donor-acceptor recombination as well as the wide PL band near 600 nm small intensity, which is due to the presence of deep acceptor centers. The nature and energy levels of defects in the CdS:Dy thin films are discussed. For the films obtained at T_s> 450 C the PL spectra include the intense broad band near 600 nm but the emission in the exciton region absent. Thus, the obtained results let us to determine the optimal conditions the preparation of the investigated thin films of excellent optical quality.

Radiation Defects in Multilayer Structures

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It is known that the effects of radiation on semiconductor materials is manifested in the change of their electrophysical and recombination, optical and many other characteristics [1]. For the observed effects, responsible as the primary processes of formation of elementary defects (vacancies and interstitial atoms), and secondary processes, which consist in the formation and accumulation of complexes of simple defects with impurities or other imperfections of the lattice of crystals. It is known that the processes of radiation defect formation are greatly influenced by various factors. The efficiency of formation and annealing of certain radiation defects (RD) depends on the availability of active and inactive uncontrolled impurities, their content and condition in the lattice of silicon, the type of dopant, its concentration, the presence of multiple contaminants and many other factors.

In this work we studied the transformation of radiation defects in silicon multilayer structures, such as the TIR and the MOSFETs. As shown by the results of the numerous experiments, these devices are extremely sensitive to radiation.

The increase of doses of irradiation of gamma-quanta 60Co MIS structures leads to a shift of C-V characteristics towards negative voltages, which indicates the appearance of radiation defects at the interface Si-SiO2. It is shown that at high radiation doses stable inversion layer at the silicon surface is not formed, since the capacitance decreases with increasing negative bias to the field electrode structure. This distortion of the inversion layer associated with the appearance of a through current in the order of 10-8 and through the oxide.

Using the method SS-DLTS revealed the formation of typical RD at the interface Si-SiO2 in the volume of the dielectric and in the bulk of the silicon separately. It is established that the appearance of the peak of the SS-DLTS near 302 K due to the presence of dangling bonds on the silicon atom. Therefore, our experimental data can be interpreted as the effect of the spatial distribution of such defects in the transition layer between silicon and oxide.

On the basis of this research, we propose a qualitative picture of the electronic processes occurring in the Si-SiO2 system after the pulse of positive polarity on the metal electrode of the MOS structure.

[1]. The issues of radiation technology of semiconductors. / Ed.by L.S. Smirnov, N., 1980, p. 294.

Spectroscopic Study of Both Quasiperiodical Microrelief and Metal Nanowires Induced Photocurrent Enhancement in Surface Barrier Solar Cells

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Surface texturing is known as an effective method to enhance solar cell (SC) efficiency via reduction of optical losses caused by the light reflection and absorption in metal contact electrodes. The elaborated technology allowed us to prepare quasiperiodical microrelief with intended parameters variation at (100) surface of n-GaAs. An alternative method of the optical losses reduction is to use metal nanoparticles or periodical array of nanowires for excitation of surface plasmons (SP) or evanescent waves-surface plasmon polaritons (SPP). To investigate the possibilities of the solar cell photocurrent enhancement by joint effect of these methods we use the formerly determined method of forming plasmonic metal (Au) nanowires on the ridges of GaAs surface microrelief during the deposition of Au from corresponding salt solution.

Parameters of microrelief (mean period and depth of grooves) were determined by AFM technique and used in the theoretical modeling for calculation of optical (transmittance, reflectance and absorption) spectra for *p*- and *s*-polarized light. Measurement of the SC short-circuit photocurrent spectra and the light current-voltage characteristics under AM0 simulated illumination showed that photocurrent enhancement caused by microrelief with predetermined parameters can reach from 2 to 10 in different spectral range due to Au nanowires deposition.

Theoretical modelling and experimental investigation of spectral, photoelectric and electricalcharacteristics of these structures allowed us to determine physical mechanisms of the photocurrent enhancement effect and its dependence on geometrical parameters of microrelief and nanowires controlled with technological regime.

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Optical Properties and Stability of Double-Layer Rubrene-Alq3 Films Fabricated by Vacuum Deposition

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Being the organic semiconductor with the very high carrier mobility reaching 40 $cm^2V^{-1}s^{-1}$, major applications of 5,6,11,12-tetraphenyltetracene (rubrene, Rub) are organic light-emitting devices (OLED) and field-effect transistors. Rub is also used as a dopant to enhance the efficiency and stability of organic thin film electroluminescent devices. Rub was reported [1] to be used in tris(8-hydroxyquinolinato)aluminium (Alq3)-based OLEDs to improve their operational parameters by reducing the formation of unstable Alq3 cationic species [2]. However, the stability of Rub itself in such devices is rather questionable because of its chemical instability and easy degradation due to the photo-oxidation. Therefore it is necessary to get better understanding of the underlying phenomena which determine Rub practical application in basic devices. In this report we present the structure, morphology and photoluminescence (PL) properties of double-layer Rub-Alq3 films deposited on freshly cleaved KBr or atomically smooth Au(111) surfaces by vacuum deposition method. Stable vacuum deposition behaviour of the both compounds was confirmed with FTIR spectroscopy (Bruker IFS-88, 2cm^{-1} resolution, 64 scans). The morphology of the structure of the first near-surface layers of Rub deposited on atomically flat Au(111) surface as investigated with STM method, which reveals molecular Rub rows preferentially oriented along (112) direction of the Au(111) substrate. Our main attention was focused on the role of Alq3 coverage on optical properties and stability in the fabricated structures. By monitoring in time the evolution of PL emission, we found that the Rub degradation in Rub-Alq3 films occurs slower than that in vacuum deposited single layer Rub layers. These results demonstrate that the deposition of Alq3 layer could insignificantly enhance the stability of Rub to photo-oxidation in optoelectronic devices.

[1]. Z. Zhang, X. Jiang, S. Xu, T. Nagamoti and O. Omoto, The effect of rubrene as a dopant on the efficiency and stability of organic thin film electroluminescent devices //J. Phys. D. -1998.-V. 31.-No.1.-p. 32-37.
[2]. Z.D. Popovic, H. Aziz, N. Hu, A. Hor and G. Xu, Mechanism of the intrinsic (long-term) degradation in Alq3-based organic light emitting devices, Proc. SPIE. - 2000.- V. 3797. - p. 310-313.

Citrate-Mediated Surface Properties of Hydroxyapatite: Hydrophilicity and Structure of {01-10} Crystal Facets

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Bio-inspiration approach to design of synthetic materials for substitution of biological ones is among the principal concepts directing innovation in the field of biomaterials. In this respect, synthetic crystalline nanoparticles of hydroxyapatite (nano-HA) prepared in the presence of citrate ions appears to be a relevant subject, since its structural features and chemical composition resemble the mineral phase of calcified biological tissues.

Observation of nano-HA samples maturated at 4, 24, and 96 hours with High-resolution transmission electron microscopy evidenced elongated along c-axis and mostly limited by {01-10} facets shape of nanoparticles. Further, the structure and properties of this most abundant surface was studied by IR spectroscopy in controlled atmosphere, microgravimetry, and microcalorimetry.In particular, combination of in-situ IR probing of surface by CO with theoretical data obtained from the modelling of vibrational behavior of CO on nano-HA surfaces of particular structure provide us with the idea of the surface structure of the real nano-HA particles. This approach allowed to reveal the overall domination of P-rich type of structure of {01-10} surface over {01-10} Ca-rich type in a ratio reaching 20:1.

Further, energetic aspect of water adsorption on nano-HA prepared in presence of citrates in contrast to HA synthetized without any have been investigated by adsorption microcalorimetry. The values of $-\Delta H_{ads}$ are grouped in two homogeneous families: for citrate-free materials ranging from 130 to100 kJ/mol and citrate-apatite materials in range 100-80 kJ/mol indicating significant interaction of water molecules with surface adsorption sites.

Thus, nano-HA prepared with participation of citrates exhibit interesting properties comparing to similar citrate-free materials, as fine surface structure in terms of {01-10}_Ca-rich:{01-10}_P-rich ratio, quantitative and energetic aspects of water adsorption.

Computer Simulation of Optimal Ionic Treatment of Metals and Alloys Surface

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Ionic implantation is a method of introducing impurity atoms into a surface layer of a plate or epitaxial film by bombarding it with high-energy ions. As a result, the target ions penetrate the surface layer of the sample to a depth of several nanometers to several micrometers. Ionic implantation has many advantages, some of them are high bond strength of the substrate and implant material, due to the introduction of the ions to a certain depth; invariance of the shape and size of the carrier in the processing; clean process conditions, etc. It is impossible to observe the process of ionic implantation, because it passes in an enclosed space. But you can explore implanted surfaces with the help of expensive equipment, such as XRD of thin films, SEM, AFM and XPS methods.

On the other hand, it is possible to predict the results using various programs simulating the process of bombarding surface with target ions. There are a big number of programs that help in this (SPURT.MP, CALCMULT, SRIM), but we used the program "Rio" [1] as the most optimal variant. The program "RIO" allows to calculate parameters such as roughness, profile length, average angle of inclination, and so on. With the help of the "RIO" program, we can find out how many ions a certain surface area will receive after the ionic implantation process.

In some cases, there are difficulties in implanting intricate surface shape, for example, shaft type parts. The ions are distributed unevenly when the surface is bombarded. One solution of this problem is ionic implantation with a surface rotation.

Using the "RIO" program, the minimum angles between the ions flux and the tangent were found. Following the geometric calculations, we can find the required number of rotation.

[1]. Nanodimension layers on stainless steel surface synthesized by ionic implantation and their simulation/ A.A. Cherny, S.V. Maschenko, V.V. Honcharov, V.A. Zazhigalov / International research and practice conference: «NANOTECHNOLOGY AND NANOMATERIALS NANO—2014». P. 170

Optical Properties of X-ray Irradiated Cu_6PS_5I-based Superionic Thin Films

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Cu_6PS_5I crystals belong to an argyrodite family [1] and are known as superionic conductors or solid electrolytes. The physical properties of Cu_6PS_5I single crystals are well known while the investigation of thin films on their basis only begins [2]. The influence of X-ray irradiation on optical absorption edge parameters of Cu_7GeS_5I thin films was investigated [3].This paper is dedicated to the optical studies of X-ray irradiated Cu_6PS_5I-based thin films. Thin films were deposited from polycrystalline Cu_6PS_5I target onto silicate glass substrate at room temperature by non-reactive radio frequency magnetron sputtering. The structure of the deposited films was analyzed by X-ray diffraction and scanning electron microscopy (SEM) technique (Hitachi S-4300). Diffraction pattern shows the films to be amorphous. The thin films chemical composition ($Cu_{5.56}P_{1.66}S_{4.93}I_{0.85}$) was determined by energy-dispersive X-ray spectroscopy (EDX). X-ray irradiation was performed for the different exposition times (30, 60 and 120 min) using wideband radiation of Cu-anode X-ray tube with approx. 400 W of power applied (33 kV, 13 mA). Optical transmission spectra of Cu_6PS_5I-based thin films was studied at room temperature using MDR-3 grating monochromator. Both unirradiated and X-ray irradiated Cu_6PS_5I thin films exhibit the Urbach behavior of optical absorption edge. For characterisation of absorption edge energy position such parameter as E_g^α at a fixed absorption coefficient value α=10^4 cm^{-1} was determined. The observed variation of optical absorption edge leads to E_g^α value decrease and E_U value increase with irradiation time increase (from 2.835 to 2.655 eV and from 249 to 404 meV respectively). The Urbach energy E_U increase is the evidence of structural disordering due to X-ray irradiation. With irradiation time increase a nonlinear increase of refractive index value is revealed (from 2.443 to 2.461 at λ=1 μm).

[1]. W. F. Kuhs, R. Nitsche, K. Scheunemann, The argyrodites – a new family of the tetrahedrally close-packed srtuctures // Mat. Res. Bull. – 1979. – V. 14. – p. 241 – 248.

[2]. I.P. Studenyak, M. Kranjčec, V.Yu. Izai, A.A. Chomolyak, M. Vorohta, V. Matolin, Cserhati C., Kökényesi S., Structural and temperature-related disordering studies of Cu_6PS_5I amorphous thin films // Thin Solid Films. – 2012. – V. 520. –p. 1729 - 1733.

[3]. I.P. Studenyak, A.V.Bendak, V.Yu. Izai, A.M. Solomon, P. Kúš, M. Mikula. Optical parameters of X-ray irradiated Cu_7GeS_5I thin films // Uzhhorod University Scientific Herald. Series Physics. – 2016. – V. 37. –p. 32 - 37.

Synthesis, Structure and Spectral-Fluorescent Properties of Organic-Inorganic Perovskite $CH_3NH_3PbI_3$ Films

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Organic-inorganic halide perovskites $APbX_3$ (A – CH_3NH_3, X – Cl, Br, I) attract now extensive scientific interest as a potent photoactive matrix for solar energy harvesting [1]. These compounds demonstrate high photovoltaic conversion efficiencies in laboratory conditions at relatively low costs of production and processing, having the only major drawback to overcome, viz. low durability.

Hitherto, there are no data in the literature about the effect of the $CH_3NH_3I : PbI_2$ ratio in the starting work solution on the structure and properties of organic-inorganic films of halide perovskites $CH_3NH_3PbI_3$. In this work, the microstructure, phase composition, and spectral-fluorescent properties of thin films of this organic-inorganic perovskite deposited on a glass substrate via spin-coating and heat-treated at 80 °C or 150 °C were studied at different reagent ratios in the initial solutions.

The shape and particle size of the films depend strongly on the reactants stoichiometric ratio. When the $CH_3NH_3I : PbI_2$ ratio is 1 : 1, the film consist of needle-like particles located along the substrate plane. For the ratio 2 : 1, the round-shaped particles were obtained. With the further increase of methyl ammonium iodide content (3 : 1), a smooth transition from round to polyhedral particles was observed. In all three cases, the $CH_3NH_3PbI_3$ particles are predominantly located in a single layer.

It is found that as the CH_3NH_3I content increases, the UV/Vis absorption spectra become more selective – the intensity increases in the region of 350-400 nm while the absorption in the visible spectrum range decreases. In the initial solution in DMF, the absorption range does not exceed 350 nm, with the most long-wavelength band at 327 nm indicating partial complexation of the mixture components in solution. Relative fluorescence intensity of the studied $CH_3NH_3PbI_3$ films increases with the higher content of CH_3NH_3I in the initial solution. This regularity is observed for films after heat treatment at both 80 °C and 150 °C, although in the latter case the fluorescence is abated substantially, probably because of partial destruction of perovskite [1].

[1]. Y. Zhao, K. Zhu. Organic–inorganic hybrid lead halide perovskites for optoelectronic and electronic applications // Chem. Soc. Rev. – 2016. – V. 45. – N. 3. – p. 655 – 689.

Spectroscopic Analysis of Molecular Photodissociation in NH_3 Thing Films

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Bond breaking by selective excitations of core electrons is an interesting field of desorption induced by electronic transitions. Core orbitals are well localized allowing allocation of the primary excitations to distinct atoms of the substrate-adsorbate complex, and core excitations very efficiently drive dissociation and desorption. Upon decay, Auger or autoionization electrons are emitted as clear signatures of the decay route and the sequence of core-excited and valence-excited states, and the well-known lifetimes of the core holes give access to details of the reaction dynamics. The possibility of allocating the excitations to distinct atoms enables the study of resonant energy transfer processes [1]. For thing solid films NH_3/Ru(001) strongly enhanced H^+-emission was found for excitation of 1s electron into strongly antibonding LUMO levels [2]. To restore whole energy relaxation scheme, it is necessary to measure simultaneously yield curves of charged and neutral species.

All measurements were performed at the BW3 beamline of HASYLAB at DESY in Hamburg. The photon flux was about 10^{12} photons/s. The Ru(001) substrate was cleaned by Ar^+ sputtering, heating in oxygen, and annealing, and the cleanliness was checked by X-ray photoelectron spectroscopy (XPS) and near edge extended X-ray absorption fine structure (NEXAFS). To analysis of the spectra of photostimulated desorption (PSD) of neutral molecular fragments and to reveal those energy ranges of molecular dissociation photoexcitation at which the branching of energy relaxation paths occurs, all PSD-spectra were normalized by electron partial yield spectra [3]. Comparison of PSD spectra for H^+ and NH_2^0 allows to conclude that the true ultrafast dissociation channel, which is very pronounced in isolated molecules, is in fact not important for PSD from solid film.

[1]. P. Feulner, R. Romberg, S.P. Frigo et al. Recent Progress in the Investigation of Core Hole-Induced Photon Stimulated Desorption from Adsorbates: Excitation Site-Dependent Bond Breaking, and Charge Rearrangement // Surf. Sci. – 2000. – V. 451. – P. 41 – 52.

[2]. A.N. Ogurtsov. Cryocrystals Modification by Electronic Excitations. – Kharkiv: NTU "KhPI", 2009. – 368 p.

[3]. A.N. Ogurtsov, O.N. Bliznjuk, N.F. Kleshchev Molecular Photodissociation Analysis of NH_3/Ru(001) Films in Radiation Technology of Functional Layer Modification by Irradiation // Chem. Ind. Ukr. – 2015. – N. 4. – P. 19 – 22.

Influence of Al Film Thickness on the Surface Plasmon Resonance in the Planar Metal Nanostructures "2D-Monolayer of Au Nanoparticles / Al Film"

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In present work, westudy the absorption spectra of the following nanostructure: monolayer of gold nanoparticles with a diameter of 90 nm on a glass substrate covered by aluminum film of variable thickness in the thickness range of 0 – 55 nm. We extracted the SPR peak from the total absorption spectrum of gold nanoparticles and determined its spectral characteristics such as the total intensity, spectral position and half-width. It was obtained that an increase of Al film thickness leads to 18 nm red (low-energy) shift of SPR absorption peak. We also observed monotonic dependence of the total intensity of the plasmon absorption peak on the thickness of Al film. It was obtained that minimal absorption observed at the film thickness of about 35 nm. Another effect related to the change of the film thickness of aluminum is an increase of the half-width of plasmon absorption peak in 2.3 times.Red shift and broadening of plasmon absorption band with increasing aluminum film thickness are caused by increase of interaction between the local surface plasmon in gold nanoparticles with Al film that leads to the excitation of the surface plasmon polaritons in the metal film by the field of SPR in Au nanoparticles.

Non-monotonic behavior of plasmon absorption peak intensity at the change of Al film thickness, in our opinion, can be explained as follows. Between gold nanoparticles and aluminum film is no dielectric layer, so an existence of the electrical contact between metal nanoparticles and metal film leads to non-radiative damping of plasmon oscillations in Au nanoparticles. At small thicknesses the Al film is an island-like one, and the respective non-radiative losses are weak. At the increase of Al film thickness the losses increase that leads to increase of SPR damping and, respectively, to the decrease of SPR extinction peak magnitude. At sufficiently large thickness (larger than about 35 nm in our case), when the Al film is continuous, these losses further do not increase and SPR magnitude reaches its minimum. Meanwhile, further increase of Al film thickness leads to rise of efficiency of SPP excitation in Al film the in accordance with above considerations leads to increase of SPR extinction magnitude. Such physical processes lead to non-monotonic behavior of bare Au NPs' SP extinction peak magnitude with variation of Al film thickness.

Ellipsometric Properties of Thin Films of Highly Conductive and Transition Metals without Excitation and with Excitation of Surface Polaritons

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Ellipsometric study of thin films of various metals showed the following. For ultrathin films with the thickness of one - few angstroms the dependence of ellipsometric parameters tgΨ and cosΔ on the angle of incidence of light on the sample for each and every film was similar to the same dependence for the pure dielectric substrate. The only difference was that at the Brewster angle for thin metal film the angular dependence of tgΨ did not reach 0 compared to the pure dielectric substrate and the curve of dependence of cosΔ changed smoothly from -1 to +1 unlike pure dielectric substrate where the change happened abruptly. With increasing film thickness minimum on the curve tgΨ increased and was shifted towards larger angles of incidence, and at a film thickness matching the massive metal it coincided with the minimum for the main angle of incidence of light on metal also the angular dependence for the cosΔ continuously changed to the value corresponding to a massive metal. This situation occurred for any and all films with the sole difference that ellipsometric parameter values for different metals were not the same. A completely different situation occurred when the excitation of surface polaritons by Kretschmann method took place. For small thicknesses results were similar for all the films - reminiscent of the total internal reflection from a pure substrate. But with increasing of thickness for highly conductive metals Au, Ag, Cu, Al at angles of incidence of about of 42^0-45^0 on the curve tgΨ appeared narrow and deep polariton minimum which gradually decreased and disappeared with increasing film thickness, and at larger angles of incidence, there was a minimum of the main angle. For transition metals Cr, Mo, Ti, Ni, Fe and others, unlike highly conductive metals, wide minimum appeared with increasing film thickness, which does not disappear, but shift towards larger angles of incidence and gradually becomes a minimum at the main angle. Another interesting feature for transition metals is that at angles of incidence close to the angle of total internal reflection the value of tgΨ at the excitation of surface polaritons is much greater than one, which in principle, is impossible without the excitation of surface polaritons.

Oriented Growth of Dye Films on Vacuum-Deposited Polytetrafluoroethylene Layers

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The polytetrafluoroethylene **(**PTFE) layers, produced by hot friction transfer (FT) or by deposition in vacuum (VD) with rubbing with a cloth at room temperature, showed different orienting action for various organic materials. Unidirectional rubbing with a cloth produced aligned relief on the VD PTFE surface. Pentacene (PN) and several squaraine (Sq) compounds were deposited on the aligning PTFE layers and microstructured aligned polycarbonate substrate (PC) by VD. The PN and only limited Sq dyes revealed oriented structures with optical dichroic ratio up to 4. The comparatively large (diameter 100 nm, 15 nm high) separated round Sq crystals were grown on the FT-PTFE ridges. Smaller crystals were grown between the ridges. Sq crystals, grown on the VD-PTFE, were the same on the ridges and inside the grooves. The VD layer led to formation of much more uniform Sq film with smaller crystals. The more nuclei of the Sq on the VD-PTFE showed, that interaction between Sq molecules and VD-PTFE is stronger, than between Sq and FT-PTFE**.** The PTFE layer thickness and growth temperature influence the anisotropy of organic films deposited on it. An optimal PTFE layer thickness is 40-50 nm with grooves width about 40 nm. Sq film grown on a PC surface showed a small dichroic ratio with absorption band at ~760 nm, prevailed for parallel polarization of light in respect to the groove direction. From optical spectra was concluded, that Sq molecules inside J-aggregates preferably oriented along PC grooves, while macroscopically the crystals oriented across the grooves. The molecular orientation was the same as on PTFE layers, but with another kind of aggregation.

Structural Characteristics and Model Rheological Parameters of n-Hexadecane Wall-adjacent Layer

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Influence of solid surface on interphase liquid layer leads to formation of a special epitropic-liquid crystal (ELC) state near the substrate. ELC physical properties are significantly different from the bulk liquid. To describe the transport phenomena in ELC we improved the structural-rheological model, which was proposed in [1]. Due to the additivity of viscosity the interlayer viscosity coefficient η was determined by linear superposition of the viscosities of an isotropic liquid η_{vol} and a structured phase η_s:

$$\eta = \eta_{\boldsymbol{s}} \cdot \boldsymbol{s} + \eta_{vol}(1 - \boldsymbol{s}\ ) = (\eta_{\boldsymbol{s}} - \eta_{vol}) \cdot \boldsymbol{s} + \eta_{vo\boldsymbol{l}}\,,$$

here $\boldsymbol{s}$is the relative part of the more viscous structured phase.

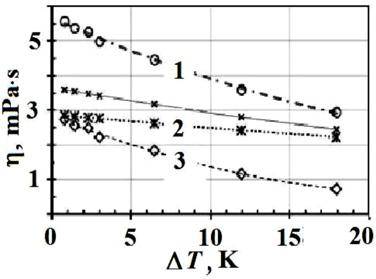

Fig. 1. Temperature dependence of different contributions to the viscosity of *n*-hexadecane interlayer

1 – ELC layer viscosity η, 2 – $\eta_{vol}(1-\boldsymbol{s})$ “isotropic” component, 3 – $\eta_s \cdot \boldsymbol{s}$ “highly-viscous” component, (×)- bulk liquid η_{vol}

The fluid flow "cuts off" the ELC layer, so its stationary thickness depends on the shear strain rate γ, taking the maximum value in the absence of flow $\boldsymbol{d}_{0s}=\boldsymbol{d}_s(\gamma \to 0)$. An inaccuracy of the extrapolation is due to the difficulty in rheological measuring at extremely low shear rates.

That is why the equilibrium thickness of ELC layer $\boldsymbol{d}_{0s}(\Delta \boldsymbol{T}=\boldsymbol{T}-\boldsymbol{T}_m)$, ($\boldsymbol{T}_m$ is the melting point of the crystal), was determined by independent optical methods, such as the measurement of induced birefringence and impurity absorption dichroism. Assuming that the rheo-parameter $\boldsymbol{s}$ is an analogue of the orientational order parameter $\boldsymbol{q}$ of liquid crystals, its measurement by independent optical methods makes it possible to estimate the contributions of isotropic and high-viscosity component to the total viscosity of the liquid interlayer.

[1] Altoiz B.A., Kirian S.V. Journ. of Eng. Phys.and Thermophys. 2010, **83**, 3. p. 608.

Thermodynamic Properties of Orientationally Ordered Wall-adjacent Liquid Layers

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According to the degree of mesogenity organic liquids are usually conditionally classified into 3 classes, such as **thermotropic liquid crystals** with high degree of molecular mesogenity (molecular shape – anisometric sphere-cylinders or flat discs); **isotropic liquids**; which are not able to form mesophase under any conditions due to low degree of molecular homogeneity and liquids which are able to form orientationally ordered state in the wall adjacent layer (WAL)under the action of solid substrate. As this layer is similar to liquid crystal it is called epitropic liquid crystalline state.

In this paper framework of we used early developed theoretical model (called “two-component” [1-2]) for numerical calculation of the temperature dependencies of equilibrium ELC layer thickness $\boldsymbol{h_s(T)}$, its specific heat $\boldsymbol{C_p(T)}$ and latent molar heat of phase transition ELC-bulk liquid $\boldsymbol{q(T)}$ with further comparison with experiment. This model postulates the existence of both monomers and dimers in the wall-adjacent layer, and the appearance of ELC layer is caused by the orientational interaction between these liquid particles and the solid substrate. The calculations were compared with results of experimental investigation of thin nitrobenzene interlayer symmetrically bounded by quartz substrates.

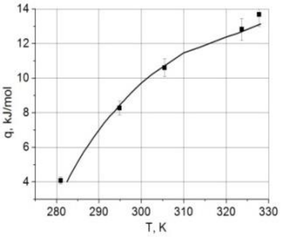

Fig. 1

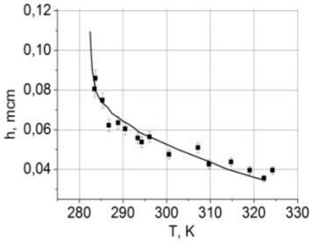

Fig. 2

In Fig. 1 and 2 it is shown that the calculated dependences (solid line) satisfactorily describe the experimental results [3].

[1]. Popovskii A.Yu., Kuznetsova A.A., Mikhailenko V.I. Adv. in Col. and Interface Sci. 2003, p.285-292.

[2]. Popovskii A.Yu., Kuznetsova A.A., Mikhailenko V.I. J. Mol. Liq. 2005,**120**, p.127-130.

[3]. Altoiz B.A, Popovskii Yu. M, Physics of wall-adjacent layers Odessa, Astroprint, 1995. – 153p. (in Russian).

Iron Titanate Films as Versatile Photocatalysts Under Solar Light

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Widespread use of semiconductor photocatalysts for environmental purification of toxic organic compounds and heavy metal ions in the waste water, drinking water and air is caused by the need to create the new nanomaterials with high surface area, define structure and high activity under both UV and visible light irradiation leading to the solar energy utilization. TiO_2, Fe/TiO_2 and N/Fe/Ti films are synthesized by sol-gel method and characterized by SEM, XRD and UV-Vis spectroscopy. The multicomponent Fe/TiO_2films treated at 450-600°C was crystalized forming the pseudobrookite structure (Fe_2TiO_5) with landauite ($Fe_2Ti_2O_7$) impurities. Band gap energy and the position of the flat band potentials of TiO_2 and Fe/TiO_2 electrodes produced by precursor coating on the titanium plates are estimated by photoelectrochemical measurements. An anodic shift of the flat-band potential position in comparison with unmodified TiO_2 electrodes is noted. High photocatalytic activity of the film under visible as well as UV irradiation correlates with the high adsorption capacity of the films treated at 450 °C. As shown by X-ray photoelectron spectroscopy, the use of urea in the synthesis procedure facilitated the nitrogen incorporation in the semiconductive structure in the form of interstitial atoms; accumulation of metal ions on the surface of nanomaterials as a result of complex compound formation during sol aging. An acceleration of crystallization rate of the photocatalytic active phase and formation of adsorption sites leading to the increased photocatalytic activity. The formation of landauite ($Fe_2Ti_2O_7$) and pseudobrookite (Fe_2TiO_5) phases at relatively low temperature (450°C) without crystallization of individual metal oxides is fixed.

N/TiO_2, N/Fe/Ti, Fe/Ti films can be recommended as versatile photocatalysts under solar irradiation due to their high photocatalytic activity of under both UV and visible light as proven by photocatalytic investigations of dichromate ions reduction and tetracycline hydrochloride degradation.

Dye Lasing in Two – Dimensional Nanoscaled Waveguides

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Dye lasers based on nanoscaled films are attractive for applications in optical communications and optoelectronic integrated component. For their fabrication two important problems should be solved: increase of concentration barrier of the dye luminescence quenching and create waveguide conditions for lasing radiation. It is need for better pumping of extremely thin films and for loss minimization of laser radiation what significantly influence the laser performance.

The first problem was solved by fabrication nanoscaled (200 nm) sol-gel films with nanopores of about 10 nm diameter filled by micelle solution of dye (rhodamine 6G). Controlling dye molecules locations allowed increasing their concentration several orders without reducing the quantum yield of luminescence. Other problem was solved by manufacture of the film based on titanium dioxide which refractive index (n=1.68) exceeds the same parameters of adjacent media. Analogous film was fabricated with SiO2 (n=1.45) which formed one-side waveguide for comparative test.

The films were pumped by the second harmonic YAG-Nd Q-switched laser whose beam was focusedin the strip 18x0.1mm^2. The radiation of the both films consisted of high divergent beam coming out of the end of the strip and two symmetrical beams coming out of her side surfaces at an angle 30^o to the film. These beams form symmetrical bands on the screen, the shape of which depends on the refractive index of the matrix. The spectrum of an axis radiation in the central beam narrows sharply from 50 nm to 4 nm and shows weak equidistant spectral lines when pumping intensity exceeds certain threshold. The spectrum widens (up to 14 nm) and lines become weaker in the peripheral part of the beam. The spectrum of lateral beams narrows substantially less, contains no lines and its shape is close to the spectrum of the peripheral part of the central beam.

Thus, we observed lasing of the films appearing as central beam radiation. This radiation consists from amplified luminescence and lasing that occurs owing to the distributed feedback of gain grating created by the oncoming waves of the amplified luminescence. Two order reducing of the lasing and changing the shape of lateral beams under changing TiO_2 matrix instead SiO_2 one is evidence of formation the waveguide amplifier in the TiO_2.The results demonstrate the possibility of waveguide lasing of the nanoscaled films.

Ellipsometric Characteriation of Si Plates Subjected to Femtosecond Laser Irradiation

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Optical properties of non-treated silicon plates and Si plates modified by femtosecond laser irradiation have been investigated by ellipsometry. The samples of the nanostructured silicon as isolated cells were formed on the single-crystal silicon wafers by a method of the laser ablation. The laser source was a home-built Yb-doped fibre laser, operating at a central wavelength of 1060 nm and generating pulses with up to 1 mJ energy at 1 MHz, which can be compressed to 100 fs. The powers incident on the samples ranged from 100 mW to 1 W. The pulse-to-pulse power stability was on the order of 0.05% (measured from 3 Hz to 250 kHz). Laser beam scanning modes provide the synthesis of nanostructured silicon dioxide particles or silicon nanoparticles. The ellipsometric parameters of the samples such as a $\cos\Delta$ and $\mathrm{tg}\Psi$ were measured by a laser ellipsometer LEF-3M-1 with $\lambda = 632.8$ nm for two mutually perpendicular directions in own plane of the sample for characterization of opticalanisotropyof silicon samples. The angular dependencies of ellipsometric parameters $\cos\Delta$ and $\mathrm{tg}\Psi$ of nanostructured silicon were analyzed and the principal angle of incidence ($\cos\Delta = 0$)and minimal value of the $\mathrm{tg}\Psi$ are obtained from these dependences.

It was established that the principal angle of incidence for nanostructured silicon is significantly reduced as compared with the one for monocrystalline silicon wafers of 12-21°. Moreover, it was found that the difference between the significance of the principal angle of incidence and the angular position of minimal value of $\mathrm{tg}\Psi$ for two mutually perpendicular directions in own plane of the nanostructured siliconis essential value equal to about 9° and more than 15° respectively. The essential difference between the values of the $\cos\Delta$ and $\mathrm{tg}\Psi$ for two mutually perpendicular directions in own plane of the sample when measured at one angle of incidence $\varphi = 53°$ was observed too. This means that the formed silicon nanostructures possess great optical anisotropy as a result of deformation influence on surface structure and appearance of elastic stresses on the surface layer of the nanostructured silicon. The optical anisotropy was not found for the silicon non-subjected areas located between the cells of nanostructured silicon.

The Structure of SiC Samples in X-Rays

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The purpose of research – the definition of the relationship between the characteristic of granules of the plates made of silicon carbide and by the closeness of their material for development of methods of control of quality of plates.

Modern protective elements modules are often composite structures. They contain layers of ceramic. Quality control of products is performed usually by measuring their density. This method does not exclude the products have the local areas to the existence of residual stress or phase or structural heterogeneity. This possibility has led to the need to determine the relationship between the parameters of spectroscopic analysis of the structure of SiC products in X-rays and density of products. For measurements, we used samples of rectangular shape with a thickness in the range of 11 - 15 mm with a content of SiC is 85-95% and Si – 5-15% When performing research usingself digital X-ray diagnostic complex «08- Alpha», X-ray spectroscopy and X-ray flaw detection methods. The researches have shown the presence of granules similar structures in products with SiC. Research performed with methods of x-ray deflectometry shown 1) that products made of silicon carbide obtained as a result of chemical reactions have internal structure in the form of granules, 2) in products containing SiC-85-95% and Si - 5-15% the size of the granules are between 0.2 - 3 mm., 3) contrast X-ray of images depends on the density of the material - with increasing sample density SiC the contrast of the image decreases.

Laser-induced Incandescence of GaSb/InGaSb Surface Layers

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Thermal emission of surface layers of light-absorbing materials under powerful pulsed laser irradiation (laser-induced incandescence, LII) is observed in the visible spectral range with the use of nanosecond-scale laser pulses. Under such laser irradiation, transient local temperatures of laser-heated surfaces reach thousands of kelvins, and the time length of LII optical signals is of the order of laser pulse duration. To a naked eye, LII looks like luminescence, however, its response on the variations of laser power is extremely non-linear (at a fixed wavelength, LII intensity, I_{LII},depends on the laser intensity, F, as $I_{\mathrm{LII}}=\mathrm{Const}*F^{\gamma}$, where the parameter γ typically changes from 3 to 10).

Thermal emission of surface layers under powerful pulsed laser irradiation can be modeled with the use of the thermal conduction equation together with the equation of transport of laser radiation and with Planck's blackbody emission law. The simulations [1] show that the intensity of LII depends on the thermal conductivity of the irradiated surface; hence LII can be applied for mapping the surfaces with hidden inhomogeneities. In the present work we demonstrate the experimental confirmation of the above-mentioned prediction.

The experiments were performed with the use of Quanta-Ray Pro-230 YAG:Nd laser operating at the third harmonic (pulse duration 6 ns, pulse energy approx. 300 mJ). LII was detected with the use of a CCD camera.

The experiments show that LII of surface layers of GaSb/InGaSb is sensitive to the concentration of In atoms. As is shown in [2], partial substitution of Ga by In in GaSb crystals causes the decrease of the crystal thermal conductivity, which affects the LII intensity as is observed in the experiments.

[1]. M.Kokhan, I.Koleshnia, S.Zelensky, Toru Aoki On the possibility of visualization of undersurface submicron-sized inhomogeneities via laser-induced incandescence of surface layers // Proc. SPIE 10097, High-Power Laser Materials Processing: Applications, Diagnostics, and Systems VI, 100970G (February 22, 2017). DOI:10.1117/12.2253006.

[2]. V. Nirmal Kumar, M. Arivanandan, T. Koyoma, H. Udono, Y. Inatomi, Y. Hayakawa Effects of varying indium composition on the thermoelectric properties of $In_xGa_{1-x}Sb$ ternary alloys // Appl. Phys. A. – 2016. – V. 122. – p. 885 – 893. DOI 10.1007/s00339-016-0409-9.

Ellipsometric Diagnostics of Ge Film on Si Substrate Subjected by Laser Irradiation

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The aim of this work consists in the characterization of Ge films on Si substrates after action of laser-induced shock waves. A laser ring pattern at the sample layer was formed to laser excite focusing shock waves. Each ring had a 200 μm diameter. The changes of surface morphology after shock wave propagation were controlled by atomic force microscopy. The selected shocked regions of the sample which included several such rings on Ge films were controlled by ellipsometrically within incident laser beam (λ=632.8 nm) using angular as well azimuthally oriented at 3 angular positions, along p-plane (placing initial measurement as 0°), at 45° orientation of sample relatively to p-plane, and perpendicular (90°) to this plane. The angular dependences of the ellipsometric parameters such as phase shift □ between the orthogonal components of the polarization vector and azimuth □ of the restored linear polarization were obtained using a laser ellipsometer ЛЕФ-3М-1. From these dependences, the principal angle of incidence ϕ0 ($\cos\Delta$ = 90°) and angular position of minimal value of the azimuth Ψmin were obtained. It is found that after action of the focused laser shock waves, weak optical anisotropy arises. The measurements Ψ and Δ as well ϕ0 and the angular position of tgΨmin in condition where longitudinal raw of unshocked "points" lies in p-plane (measurement in so-called positions 1-3 where mark 1 is a position range of the sample when it was not subjected to any laser irradiation) indicates no changes for ϕp for all 1-3 points within measurement accuracy of ellipsometric parameters. For 3 and 4 "points" it is sharply seen that more than 0.4° difference of ϕ0 relatively to 1 reference "point" is observed. After azimuthal rotation of sample in own plane of 45° for the same "points" the analogous tendency is observed although the absolute values ϕ0 are somewhat overestimated in comparison to data for 2-4 "points" orientation. For 2″, 3″ and 4″ sample positions where its orientation in own plane is changed up to 90°□ all values ϕ0 become essentially more relatively to ones for initial position 1 up to 0.2°. These results indicate that after laser treatment in the above-mentioned manner the shock-induced optical anisotropy within range of irradiation arises and may be accurately determined by angular and azimuthal ellipsometric measurements.

8

Theory

Examining the He-He Bond in Endohedral Fullerene He_2@C60: Tip of Iceberg

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> "Scientific theories are explanations: assertions about what is out there and how it behaves."
> David Deutsch 'The Beginning of Infinity'

Twenty years have already been passed since the endohedral fullerene's void ceaselessly attracts attention of both, experimentalists and theoreticians, computational chemists and physicists in particular, who direct their efforts on computer simulations of encapsulating atoms and molecules into fullerene void and on unraveling the arising bonding patterns. This work begins with a survey of the recent developments on the endohedral $Ng_2@C_{60}$ fullerenes with two encapsulated **n**oble-**g**as atoms, on their experimental observation and on related computational works. The two latter are the main intrigue of the work: on the one hand, there experimentally exists the He dimer embedded into C_{60} void: otherwise, C_{60} void of 7.14 Å diameter is not enough to encapsulate two neutral He atoms due to the experimental averaged bond length of He_2 dimer amounts to 52 Å [1]. On the other, computational side, each He atom exhibits a negligible charge transfer to C_{60} resulting in that altogether, that rules out, relying on the classical chemical definition of a bond [2], any bond formation between two He atoms. This work critically examines various approaches and shows that the He dimer exists inside C_{60} as a fractionally charged $(He^{+\delta})_2$, $\delta \approx 0.01$ e. We propound a formation of the He dimer in a given C_{60} void by largely focusing on the He-He potential energy well which was scanned and analytically approximated. It is demonstrated that this well is deep enough to maintain at least one bound (ground) state. According to Löwdin's postulate of a molecule [3] which naturally is anticipated within quantum theory, we infer that $(He^{+\delta})_2$ is a molecule, a diatomic, where two heliums are bonded to each other. Since a bond is a two-body creature, we conclude that it suffices to define a bond on the basis of Löwdin's postulate which we also extend on the concept of stability of endohedral fullerenes.

[1]. J.P. Toennies. Helium clusters and droplets: microscopic superfluidity and other quantum effects// Mol. Phys.-2013.-V.111.-N.12-13.-p.1879-1891.
[2]. A.D.McNaught,A.Wilkinson. IUPAC Compendium of Chemical Terminology (the "Gold Book"). Blackwell Scientific Publications, Oxford, 1997.
[3]. P.-O. Löwdin. On Nuclear Motion and the Definition of Molecular Structure.// J. Mol. Struct. (Theochem).-1991.-p.13-15.

Statistical Cell Model of Ternary Solutions Applied for Determining the Interaction Energy Between Two Molecules

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The spectral shifts of some azo-dies absorption bands recorded in ternary solutions achieved in binary solvents having one active and one inactive (from intermolecular point of view) components are analyzed based on the statistical cell model for ternary solutions and the difference between the interaction energies in molecular pairs of the types azo-dye-active solvent and azo-dye inactive solvent is estimated.

In solutions in which specific interactions take place, the adequate choose of the binary solvent permit us to estimate the strength of the hydrogen bonds realized between the protic solvents and the spectrally active molecule.

Spectral Particularities of Femtosecond Optical Pulse Propagating in Dispersive Medium

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Ultra wideband optical signal propagation through the dispersive medium have been studied for tens years. The origins of this problem date back to Somerfield and Brillouin. They studied propagation of sinusoidally modulated step signal. Modern publications (see Oughstun`s books and references in it) [1] were devoted to study: step-function, δ - pulse, monochromatic optical signals, etc. We proposed to use elementary wave packets (EWP) series as physically grounded representation of ultra-short optical pulses to learn this problem [2-3].

We have solved wave equation for Lorentz Model of substance without restriction on frequency bandwidth of optical signal and spectral properties of the medium. Then we used these solutions to investigate such problems: 1) behavior of high and low frequency parts of signal; 2) parameters of so called “forerunner”; 3) velocity of the EWP-pulses including data transfer velocity; 4) femtosecond time domain spectroscopy; 5) relativistic restriction on the time delay of optical pulse propagation and complex material parameters of the medium, etc.

Some more we propose to apply EWP-series for medium dispersive properties characterization as alternative to Fourier decomposition method.

Conclusion. Ultra wideband femtosecond optical pulse source is effective instrument as for fast measurements of spectral peculiarities of substance and high density data information flow transfer.

[1]. K. Oughstun. Electromagnetic and Optical Pulses Propagation. Springer, Dordrecht, Volumes 1, 2: (2009).

[2]. V. Ovechko. Femtosecond optics - optics of the elementary waves packets, J.Opt.Soc. Am. B-29, (2012), B799-B805.

[3]. V. Ovechko. Femtosecond optical pulse propagation through the single resonance Lorentz model dielectric, International J. of Advanced Research in Physical Science. Volume 4, Jan. 2017, 28-34.

Plasmon Enhanced Excitation of Molecule by Electron Energy Loss Spectroscopy

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This report shows that due to the interaction a molecule with plasmons of a metallic nanoshell, the inelastic scattering of electrons by the molecule is enhanced by several orders of magnitude. For this purpose, the quantum-mechanical theory of inelastic electron scattering by the above system is developed [1]. It is shown that plasmon assisted electronic microscopy may allow resolving images of subdiffraction-limited excitation volumes [2].

The electron energy loss spectra dependence on the energy of electrons, the angular relative position of the molecule and the particle, and the dipole moment of the molecule are presented. It is shown that the probability of the molecular excitation by fast electrons grows enough enable observation of individual molecules on the surface of the nanoshell in an electron microscope.

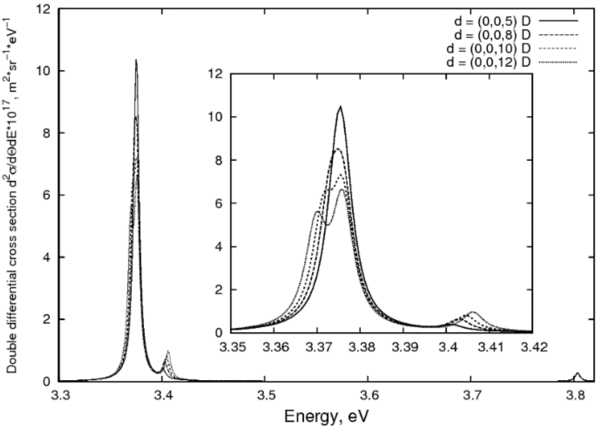

Fig. 1. Scattering of electron by a system consisting of the molecule and the nanoshell dependence on the dipole moment of the molecule.

[1]. I.Yu.Goliney, Ye.V.Onykienko // Resonant Enhancement of Molecular Excitation Intensity in Inelastic Electron Scattering Spectrum Owing to Interaction with Plasmons in Metallic Nanoshell// UJP. - 2014. - V. 59. - N. 9.

[2]. Katherine A. Willets, Andrew J. Wilson, Vignesh Sundaresan, and Padmanabh B. Joshi // Super-Resolution Imaging and Plasmonics // Chemical Reviews. - January 13, 2017.

Theory of Interparticle Interactions in Water and Alcohols of Methanol Series

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In general, the interparticle interaction in water and alcohols of methanol series is described by the potential:

$$\Phi(1,2) = \Phi_R(1,2) + \Phi_D(1,2) + \Phi_E(1,2) + \Phi_H(1,2),$$

where Φ_R and Φ_D are the terms describing the repulsive and dispersive interactions correspondingly, Φ_E is the electrostatic contribution depending additionally on the angles and which determine the orientations of molecules, Φ_H is the H-bond contribution.

An H-bond is considered as a combination of electrostatic attraction and irreducible one caused by exchange effects arising due to overlapping of the electronic shells of water molecules. It is shown, that the overlapping degree is close to zero. It means that the irreducible part of intermolecular interaction should be also close to zero.

It is evident that the simplest thermodynamic properties of the water vapor, such as equation of state, the coexistence curve and other, are determined by the averaged interparticle potential. From physical point of view, the averaging of potential is caused by rapid rotational motion of water molecules. Averaged potential has the Lennard-Jones structure.

Operating by averaged potentials allows us to formulate the generalized similarity principle. Applying this principle, we can calculate with high accuracy the critical temperatures of water and methanol, supposing that argon is basic liquid with all known properties.

[1]. M.V. Timofeev. Simulation of the Interaction Potential Between Water Molecules // Ukr. J. Phys. – 2016. – V. 61. – N. 10. – p. 893-900.
[2]. S.V. Lishchuk, N.P. Malomuzh, and P.V. Makhlaichuk. Why Thermodynamic Properties of Normal and Heavy Water Are Similar to Those of Argon-like Liquids? // Phys. Lett. A. – 2010. – V. 374. – N. 19-20. – p. 2084-2088.
[3]. I.V. Zhyganiuk, M.P. Malomuzh. Nature of the Frequency Shift of Hydrogen Valence Vibrations // Ukr. J. Phys. – 2014. – V. 59. – N. 12. – p. 1183-1190.

Photoinduced Diffusion Molecular Transport

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We consider a Brownian photomotor [1-4], namely, the directed motion of a nanoparticle in an asymmetric periodic potential under the action of periodic rectangular resonant laser pulses which cause charge redistribution in the particle. Based on the kinetics for the photoinduced electron redistribution between two or three energy levels of the particle, the time dependence of its potential energy is derived and the average directed velocity is calculated in the high-temperature approximation (when the spatial amplitude of potential energy fluctuations is small relative to the thermal energy) [5]. The thus developed theory of photoinduced molecular transport appears applicable not only to conventional dichotomous Brownian motors (with only two possible potential profiles) but to a much wider variety of molecular nanomachines. The distinction between the realistic time dependence of the potential energy and that for a dichotomous process (a step function) is represented in terms of relaxation times (they can differ on the time intervals of the dichotomous process). As shown, a Brownian photomotor has the maximum average directed velocity at (i) large laser pulse intensities (resulting in short relaxation times on laser-on intervals) and (ii) excited state lifetimes long enough to permit efficient photoexcitation but still much shorter than laser-off intervals. A Brownian photomotor with optimized parameters is exemplified by a cylindrically shaped semiconductor nanocluster which moves directly along a polar substrate due to periodically photoinduced dipole moment (caused by the repetitive excited electron transitions to a non-resonant level of the nanocylinder surface impurity).

[1]. P. Reimann. // Phys. Rep. – 2002. – V. 361.– P. 57 – 265.
[2]. M.L. Dekhtyar, A.A. Ishchenko, V.M.Rozenbaum. // J. Phys. Chem. B – 2006. – V. 110.– P. 20111 – 20114.
[3]. M.L. Dekhtyar,T.Ye. Korochkova,V.M.Rozenbaum. // Int. J. Quantum Chem. – 2010. – V. 110. – P. 67 – 76.
[4]. M.L. Dekhtyar,V.M.Rozenbaum. // J. Chem. Phys.–2011.–V. 134. – P. 44136 -4.
[5]. V.M.Rozenbaum, M.L. Dekhtyar, S.-H. Lin, L.I. Trakhtenberg. // J. Chem.Phys. – 2016. –V. 145.– P. 064110 – 12.

The Study of Warfarin-HSA Binding by Means of Molecular Dynamics Simulation

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Human Serum Albumin (HSA) is a natural protein found in the human body. It has proven preferable to artificial mediums, ideal as a stabilizer in pharmaceutical and biotech products, effective as a drug delivery vehicle, and very useful in cryopreservation and cell culture, as well as in other applications [1]. At this an understanding of the forces driving the formation of ligand-HSA complexes is still a very challenging task for molecular design. Binding event (ligand-protein binding pose and the strength of their interactions) can be predicted by molecular docking, albeit intrinsic entropic contributions and solvation effects are usually ignored.

We focus on the stability determining factors of HSA complexes with anticoagulant drug warfarin, which are examined by measuring broadband acoustic spectra [2] and by performing all-atom molecular dynamics simulations at constant pressure and in the course of structure relaxation after pressure jump [3]. We obtained a positive value of binding enthalpy for warfarin-HSA complex formation in aqueous environment and assumed that unfavorable effect due to release of significant amount of water molecules previously bound to the interacting surfaces of the ligand and receptor. Therefore we highlight the importance of the entropy contribution and the role of acceleration of water dynamics and retardation of the protein internal dynamics for the warfarin-HSA complex stabilization.

We consider totally seven molecular processes which cause conformational and solvation entropic contributions and play significant role, affecting the free energy of warfarin-HSA binding. These processes with characteristic time constants between 0.5 ps and 0.5 μs involve mobility of bulk and solvation water as well as global and local conformational changes of the protein.

[1]. P. Ascenzi, A. Bocedi, S. Notari, et. al. Allosteric Modulation of Drug Binding to Human Serum Albumin. // Mini-Reviews in Medicinal Chemistry. - 2006. – V. 6. – P. 483-489

[2]. T.Hushcha, U. Kaatze, A. Peytcheva. Dynamics of Human Serum Albumin Studied by Acoustic Relaxation Spectroscopy // Biopolymers. – 2004. - V. 74. - P. 32-36.

[3]. S.O. Yesylevskyy, T.O.Hushcha. Conformational Relaxations of Human Serum Albumin Studied by Molecular Dynamics Simulations with Pressure Jumps // Biopolymers and Cell. – 2012. – V. 28. – N. 6. - P. 486 - 492.

Pressure Effect on the Parameters of Adiabatic Potential in the Crystals of $CuInP_2S(Se)_6$ Family

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The conditions of the order-disorder phase transitions realization for the $CuInP_2S_6$ and $CuInP_2Se_6$crystals based on the adiabatic potential concept have been proposed in [1, 2]. Using the symmetry methods, the authors [1, 2] constructed the matrix of the vibronic potential energy and found the adiabatic potentials. The matrix of the vibronic interaction potential energy was built as a sum of invariants that are based on the normal coordinates Q_1, Q_2 and their combinations, which transform according to the representation Γ_5 of the space group D_{3d}^2. It was shown [2] that the vibronic interaction (cooperative Jahn-Teller effect) is a possible cause of observed phase transition due to the existence of nearby-in-energy local *d*-electronic levels, which are connected with the Cu atoms.The shape of these adiabatic potentials shows that in their conception one can confirm about the order-disorder phase transition if to consider the influence of the elastic deformation (pressure) and temperature on these potentials.

The adiabatic potentials dependence on the pressure is established by means of the modeling of the potentials dependence on the elastic deformation tensor components in the framework of the Pikus' method of invariants, which was developed for the determination of the energy spectrum versus the wave vector for the semiconductor crystals.

In this report, we analyze the effect of the linear and quadratic Jahn-Teller coupling and the strain on the adiabatic potential energy in the $\Gamma_5 - \Gamma_5$ system for the $CuInP_2S(Se)_2$ crystals. It is shown that in a consequence of the phase transition the splitting of the equivalent minima (disorder) of the adiabatic potential on the group of the nonequivalent minima (order) takes place. The Jahn-Teller stabilization energy and the distortion amplitude at the pressure change are determined. The estimations of the vibronic coupling parameters are obtained from first-principles electronic structure calculations.

[1]. D.M.Bercha, S.A.Bercha, K.E.Glukhov, M.Sznajder. Electron-Phonon Interaction as a Mechanism of Phase Transition in a Layered $CuInP_2S_6$ Crystal //Acta Physica Polonica.- 2014.- V. A 126.- P. 1143 -1145.

[2]. D.M.Bercha, S.A.Bercha, K.E.Glukhov, M.Sznajder. Vibronic interaction in crystals with the Jahn-Teller centers in the elementary energy bands concept //Condensed Matter Physics.- 2015.- V. 3.- P. 33705:1-17.

Calculated Spectra of Low Molecular Weight Hydrocarbons

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To determine the content of accompanying gases and liquids in hydrocarbons and the composition of natural gas, various physicochemical methods are used, among which the most accurate and reliable are the vibrational Raman spectra. Vibrational spectroscopy of infrared absorption (IR) and Raman scattering (RS) is used for analytical purposes: both for determining the molecular structure and for identifying substances; qualitative and quantitative analyzes of their mixtures.

Raman spectra of natural gas (NG) in the range $500 \div 3500\ cm^{-1}$ of combinational frequencies under normal conditions are studied. The results of the studies show that the region of stretching vibrations of C-H hydrocarbon bonds, despite the very high level of the Raman signal, is of little use for quantitative and qualitative analysis. This is since the structure of the bands in this region of the spectrum is very complex and the methane bands with its suppressing content in the NG dominate here [1 - 3]. The spectra of weak bands of heavy hydrocarbons against the background of very intense bands of methane are almost not released. In full, to consider all the details, as can be seen from the previous one, it is difficult.

Therefore, we paid special attention to the determination of the molecular components of NG methane (CH_4), ethane (C_2H_6), propane (C_3H_8) and butane (C_4H_{10}) by determining the C-H vibrations, and determining in which spectral region they are located.

The frequencies of C-H vibrations of pure ethane under conditions of an isolated ethane molecule, C-H of the pure propane vibration under the conditions of an isolated propane molecule and C-H vibrations of pure butane under conditions of an isolated butane molecule are calculated.

The results of the calculation confirm that indeed the frequencies of C-H vibrations of heavy hydrocarbons (ethane, propane and butane) lie in the spectral range of $2500 \div 3500\ cm^{-1}$ of combinational frequencies.

[1]. Bazhanov Yu.V., Vlasov VI, Vovk SM. And others // Analytics and control, №3-4, 1998. P.65-74

[2]. Buldakov M.A., Korolkov V.A., Matrosov I. I., Petrov D.V., and Tikhomirov A.A. // J.Opt. Technol. 80 (7), July 2013. PP.426-430

[3]. Kuyliev BT, Zhumaboev A., Meiliev L.O. and others. // Uzbek Journal of Physics. 2016. Vol. 18, №5. P.191-197

Degree of Dimerization and Effective Polarizability of Molecules of Liquid Water and Its Saturated Vapor

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The talk is devoted to the investigation of dielectric properties of water and its saturated vapor. The main attention is focused on the physical nature of its effective polarizability. We show that the specific temperature dependencies of these characteristics are mainly caused by thermal vibration excitations of water dimers. In connection with this we determine normal coordinates for the dimer vibrations. We investigate fluctuations of the dipole moments of dimers in details and consider their contributions to the dielectric permittivity of the water vapor. Analyzing the behavior of the effective polarizability we determined the temperature dependence of the dimer concentration on the coexistence vapor-liquid curve. The noticeable dimerization in the saturated water vapor takes place only for temperatures $t = T/T_c > 0.8$ (T_c is the critical temperature).

It is shown that the effective polarizability of a system has the structure

$$\alpha_{eff}(t) = \alpha_e + \alpha_d(t) + \frac{d_{eff}^2(t)}{3t},$$

where $\alpha_d(t)$ is the contribution arising due to vibrational excitations of dimers and $d_{eff}(t)$ is the effective dipole moment. It is established that near the triple point the effective polarizability of a molecule in liquid state tends to $\alpha_{eff} \approx 0.36$ and $d_{eff}(t) \approx 0$.This value of α_{eff} approximately corresponds to the half of dimensionless effective polarizability of a dimer. Since the effective dipole moment is practically equal to zero, we should conclude that 1) the observed value of the effective polarizability per molecule is generated by the set of dimers; 2) two neighboring dimers are in antiparallel states similar to those for tetramer; 3) three dimers can form hexamers similarly to that in hexagonal ice. In these and similar cases dipole moments are equal to zero. In liquid state water dimers are the most stable among all enumerated clusters, though all they are short-living. So, we assume that dielectric properties of liquid water can be considered as those for an ensemble of dimers. The first steps in this direction had been made in [1,2].

[1]. N. P. Malomuzh, V. N. Makhlaichuk, S. V. Hrapatiy. Water Dimer Equilibrium Constant of Saturated Vapor// Russian Journal of Physical Chemistry A, 2014, Vol. 88, No. 8, pp. 1287–1292

[2]. N. P. Malomuzh, V. N. Makhlaichuk, S. V. Hrapatiy. Water Dimer Dipole Moment// Russian Journal of Physical Chemistry A, 2014, Vol. 88, No. 8, pp. 1431–1435.

Detailed Analysis of Anharmonicity-Induced Lineshapes in Raman Spectra

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Vibrational spectra are a recognized source of information about the inner structure of molecules and solids. The important characteristics of the vibrations (either oscillators in molecules or phonons in solids) can be obtained based on the analysis of spectral positions and lineshapes of the vibrational features in infrared absorption and Raman spectra. In many cases, the harmonic oscillator approximation is sufficient to obtain good agreement of experimental and theoretical results. However, there are many cases when the coupling of different oscillators is rather strong, and harmonic approximation fails. The most known example of anharmonism-related phenomena is the effect of Fermi resonance.

We report on the systematic analysis of the influence of anharmonic interactions on vibrational spectra of both molecules and molecular crystals. The trends in the spectra occurring at the variation of anharmonic interaction strength are discussed. Influence of the value and sign of detuning between the energies of interacting states is also revealed. We also demonstrate the similarities and differences between the spectra of molecules and the related molecular crystals. In the latter case, special attention is paid to the elucidation of the role of phonon branches dispersion.

We have studied the effects of anharmonic interaction between a fundamental vibration and an overtone (combination tone) in a molecule and crystal. The detailed analysis revealed the trends of spectra variation both in molecules and solids with the change of important theoretical parameters Γ and A^p that describe the contributions of the 3rd- and 4th-order anharmonism. The theoretical approach was applied to the analysis of both spectral positions and lineshapes of vibration bands. Using the above approach, we explored the effects of anharmonism in the spectra of CO_2 molecule and CO_2 molecular crystal. It was shown that in the case of crystal this phenomenon is more complicated due to participation of the whole band of two-phonon states in Fermi resonance. The method to estimate the constants of anharmonic interactions is proposed.

Decay of Intensity Correlation Function Near Instability Point for The Process of Resonant Tunneling

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We analyze the influence of external noise on the process of the intensity correlation function *C(t)* decay in a model system that describes resonant tunneling of electrons through double barrier nanostructure. This influence is the most significant near an instability point. In our model the instability takes place in the point of the transition from the state with low efficiency of tunneling to the state with the great efficiency. It was supposed that the intensity of the incoming flow may fluctuate under the influence of an external noise both white and colored. The specific feature of the processes occurring in the vicinity of the point of instability is that their behavior differs at short and long times. This is due to the fact that there is the so called the critical slowing down in the point of the transition.

For the description of *C(t)*behavior in the regions before and after the transition there are some methods represented in literature. For example, to describe the short-time behavior, the method of a projection operator leading to the continued fractions expansion has been proposed. This method leads to the one-exponential approximation of the correlation function. The approximation called the approximation of the mean relaxation time has been proposed to describe the long-time behavior.

The methods mentioned above are approximations of a lower order compared to the more general approach, namely, the method of generalized moment expansion (or the method of double expansion (DE)), which is based on simultaneously expansion of the correlation function in high and low frequencies.

We compared the results of analytical calculations with the results obtained by numerical simulation of Langevin equation for the considered tunneling process. The calculations of the correlation functions carried out with the use of different methods allow us to conclude that in the neighborhood of the instability point, the results achieved with the use of the DE method qualitatively agree with numerical simulation. Outside the region of instability, the one-exponential approximation can be used. Directly in the instability region the abnormal behavior of the correlation function was observed both in the dependence on the noise intensity D (acceleration of the correlation function decay with increase of D), and on the noise correlation time τ (acceleration of the correlation function decay with increase of τ).

Manipulation of Atoms by the Counter-Propagating Frequency-Modulated Waves

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The frequency-modulated (FM) light wave is one of the optical instruments which provides an effective control of atoms motion since 1988 when J. Hoffnagle proposed the scheme of laser cooling of atoms in an atomic beam by FM and counter-propagating monochromatic waves [1]. We analyze the interaction of the counter-propagating FM waves with an atomic ensemble and show that such waves can confine atoms near the point where the field strength of the both waves are the same. This is illustrated in Fig. 1 where time dependence of the average coordinate ‹z› and r.m.s. deviation Δz of the coordinates of 100 Na atoms with initial velocity 10 m/s are presented. We also calculated the temperature of the atomic ensemble and found the parameters of the atom-field interaction which provide sub-Doppler cooling of the atoms. We simulate the atomic motion (two-level model of the atom-field interaction) using parameters appropriate for sodium atoms. The numerical procedure is based on the quasi-classical approach which we earlier used for simulation of the atomic motion in the field of the counter-propagating pulse trains [2].

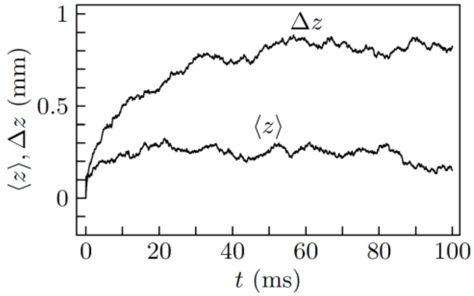

Fig. 1. Average coordinate and r.m.s. deviation of 100 Na atoms vs. time

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[1]. J. Hoffnagle. Proposal for continuous white-light cooling of an atomic beam // Opt. Lett. – 1988 – V. 13. – N. 2. – p. 102 – 104.

[2]. V.I. Romanenko, Ye.G. Udovitskaya, A.V. Romanenko, L.P. Yatsenko. Cooling and trapping of atoms and molecules by counterpropagating pulse trains // Phys. Rev. A – 2014 –V. 90. – N. 5. – 053421.

Centrosymmetrical Solitons with Power Asymptotics for Media of Different Dimensions

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The problem associated with the search for centrosymmetrical soliton-type solutions in crystals, polymers, and other nanoobjects with a nonlinear response to electromagnetic excitation was considered.

The problem is based on solving the Poisson equation for spaces with central symmetry, with a complicated power nonlinear inhomogeneity, and with trivial boundary conditions at infinity. Nonlinear inhomogeneity is the result of a series expansion. It consists of two summands, each of which contains the desired function in various powers.

A parameter was introduced into the initial equation that allows to analyze this centrosymmetrical problem simultaneously for all three dimensions: 1D (polymers), 2D (graphene etc.) and 3D (objects of crystal type).

Two branches of solutions in the form of centrosymmetric solutions are found. They are rational functions: $\varphi(r) = A/(1 + \alpha r^2)^{\nu}$, where ν is any real number $(\nu \leq 1)$. The influence on the obtained solution of the degrees of nonlinearity and the parameter determining the dimensionality of space is analyzed. It is shown that an increase in the degrees of nonlinearity in the equation leads to a decrease in the exponent ν in the solution, independently of the problem dimension. And with an increase in the dimensionality of space, the soliton tapers and its amplitude increases.

9

Methods and Applications

Speciation in Solutions of Lithium Salts in Dimethyl Sulfoxide, Propylene Carbonate and Dimethyl Carbonate from Raman Data

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Vibration spectroscopy may be considered the most powerful tool for studying speciation in non-aqueous solutions because of its sensitivity to molecular interactions between functional groups of molecules and ions.

Raman studies of cation and anion solvation and ion pairing in non-aqueous solutions of lithium salts have been performed in the concentration range from diluted solutions to the mixtures of molten solvates with salts. Solvation numbers for cations are almost independent on concentration being equal to ~2. Unlike cations, the mean solvation number of anions significantly depends on concentration and varies within wide limits.

The analysis of collision dynamics could be of great help for discerning between solvated anions, solvent separated (SSIP) and contact (CIP) ion pairs. Modulation (collision) times for free anions are short and evidence weak interactions between anions and solvent molecules. In SSIPs, τ_ω are an order of magnitude longer thus signifying strong interactions between anions and cations. In CIPs, τ_ω become shorter than in SSIPs reflecting the transformation of the structure of concentrated solutions to that of molten salts. This means that on passing from the solvated anion to the SSIP, the Raman profiles of anion lines are transforming from Lorentzian to Gaussian form, and passing from SSIP to the CIP – from Gaussian to Lorentzian form. Based on these conclusions, differences in the conductivity of solutions are explained and a conclusion is drawn that charge transfer in PC and DMC systems is carried out by SSIPs.

Application of Stimulated Raman Scattering of Lasing Dyes in Multiple Scattering Media at Room Temperature for Their Vibrational Spectrum Determination

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Stimulated Raman scattering (SRS) of lasing dyes appears in multiple scattering media (MSM) together with random lasing (RL) as a coupled process SRS-RL. Its radiation spectrum manifests all Stokes lines of Raman scattering in spectral region of RL and so may be used to determine the vibrational spectrum of dyes molecules [1]. But at room temperature SRS lines have low intensity in SRS-RL spectrum and therefore accurate separation of linear (SRS) and continuous (RL) components is need. It is especially important because of the SRS lines dependence on all the factors that influence the shape of RL contour should be account. The most important among them is heavy dependence on pumping intensity which causes the same dependence on its fluctuations. Therefore, using of accumulating or averaging methods, which are suitable for extraction of a weak signal from noise, is inefficient in this case.

We developed iterative algorithm of SRS-Rl spectrum decomposition which uses averaging of vibrational spectra independent on these factors. The algorithm processes the batch of SRS-RL spectra regardless of pumping intensity. Vibrational spectrum from each SRS-RL spectrum $I_{SRS-RL}(\omega)^n$ was determined as cubic nonlinear susceptibility $\chi_{srs}^{(3)}(\omega) \sim \ln\left(\frac{I_{SRS-RL}(\omega)^n}{\widetilde{I_{RL}}(\omega)_i^n}\right)$ which expression follows from the mechanism of SRS-RL. At i iteration decomposed RL component $\widetilde{I_{RL}}(\omega)_i^n$ is obtained using the value $\langle\chi_{SRS}^{(3)}(\omega)\rangle_i$ averaged in the previous item according to expression $\widetilde{I_{RL}}(\omega)_i^n = I_{SRS-RL}(\omega)^n \exp\left(-N_i\langle\chi_{SRS}^{(3)}(\omega)\rangle_i\right)$ which is inverse of previous relation (where i – iteration step, n – number of spectrum and N_i – pre-calculated coefficient of proportionality on i-th step). The iteration repeats until convergence.

The algorithm has been applied to a set of SRS-RL spectra of dye R6G in vesicular film at room temperature. Vibrational spectra determined from different experimental SRS-RL spectra differ slightly in the beginning from the average one. Their differences decrease with the items. Convergence occurs after ~10 iterations. The vibrational spectrum obtained with developed algorithm from SRS-RL spectra at room temperature is accurate enough and in no way inferior to the spectra obtained from the data at He temperature and by other techniques.

Influence of Multiple Scattering in the Bulk and at the Borders of Multiply Scattering Medium on the Random Lasing Characteristics

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In some approximation, the random lasing (RL) development can be represented as a formation of amplified spontaneous emission along random paths formed by multiple scattering. This approximation allows us to use the Monte-Carlo (MC) for RL simulation and for computing its characteristics depending on the parameters of the multiply scattering active medium (MSAM).

In the presented work, the distribution of the pump radiation and RL in the sample was simulated via the MC method, depending on the thickness of the MSAM, on the scattering centers concentration in it, and on the diffusive reflection rate at its borders. It is shown that spatial distributions of pump and RL radiation in a sample may be different substantially. The second one significantly depends on a sample thickness (in the direction of the pump beam incidence) and also on the ratio of bulk scattering efficiency to the diffusive reflectance of its borders.

While the pump radiation always is confined near the input surface of the MSAM, the RL radiation can be concentrated in its depth. Under the large sample's thickness the distribution of the RL density monotonically decreases deep into the sample in a manner similar to pump. With a decrease in the sample's thickness within the limits of the defined thickness being close to the photons' mean free path, the RL radiation density rises under the distance from both sample's borders increasing. In this case, the density at the maximum of this distribution also increases, and the RL threshold falls. This effect grows with the borders diffuse reflection rate increasing and disappears at a sample thickness less than the active area size.

With the bulk scattering decrease, the RL is provided by diffusive reflection at the sample's borders, what can be considered as a "photon box" which holds emitted radiation by this scattering. Growing of the borders' reflection leads to increasing the influence of the sample's sizes. Optimal RL formation occurs in the sample of such size in which the RL photons density distribution formed by the borders reflection is concentrated mainly in the active area. Exceeding of this size leads to RL propagation in the inactive area of the sample what increases the radiation losses and reduces RL effectiveness. The obtained results allow concluding that the RL efficiency can be increased by manipulation of the diffusive reflection at the sample's borders.

Photon Counting Histogram Analysis of the Scanning Fluorescence Fluctuation Spectroscopy Data

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Photon Counting Histogram (PCH)[1] method was originally developed for the analysisof Fluorescence Fluctuation Spectroscopy (FFS) data measured from a single confocal point. Based on the assumption of the dynamic system's ergodicity over time and space the PCH analysis can be applied to the fluorescence image obtained in the scanned regime. The proposed approach allows to estimate number (N) of molecules and their brightness (q) from the measured image and it has an advantage over N&B analysis[2] where only two first cumulants are taking into account. Examples of the fluorescence images are presented at the Fig. 1 (A) and the results of PCH analysis (black line) – at the Fig. 1(B). The time dependence in the PCH analysis can be well compensated using the correction for diffusion (red line).

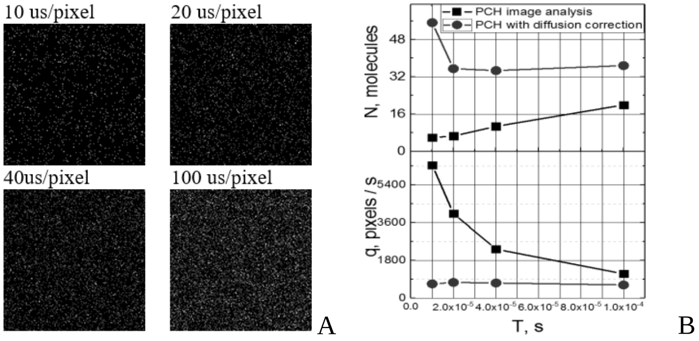

Fig. 1. Fluorescence images (a stack of 100 128x128 images) of purified GFP in buffer with various dwell time (10, 20, 40, and 100 μs/pixel) (A) and results of PCH analysis with diffusion correction (B)

The obtained values of q and N are consistent with the N&B analysis and with results from the point-FCS experiment (data not shown). Some discrepancies for experiments with 10 μs/pixel and can be explained by insufficient statistics.

[1]. Y. Chen et all.The photon counting histogram in fluorescence fluctuation spectroscopy // Biophysical. Journal – 1999. – V. 77. – P. 553 – 567.

[2]. M.A. Digman, R. Dalal, E. Gratton. Mapping the number of molecules and brightness in the laser scanning microscope. // Biophysical Journal. – 2008. – V. 94. – P. 2320 – 2332.

β-ketoenoles as Amyloid-Sensitive Fluorescent Probes for Amyloid Fibrils Detection

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Dye-based fluorescence assay is an effective technique to detect proteins and their aggregates. Amyloid fibrils are β-pleated insoluble aggregates connected with pathogenesis of neurodegenerations and amyloidosis. Thus, there is an interest in search of sensitive dyes for sensing of amyloid aggregates. Here a series of β-ketoenole derivatives with different alkylamino and aromatic substituents (Fig. 1) was studied as probes for sensing of amyloid fibrils using insulin and lysozyme as model objects. Free dyes are very weakly fluorescent; quantum yields reach up to 0.0052 values. Maxima of excitation spectra were detected within the range 362-444 nm, and fluorescence spectra maxima were detected between 496-550 nm.

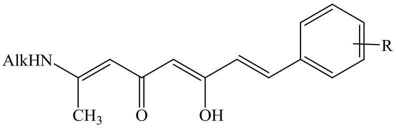

Fig. 1. β-ketoenole structure (AklHN, R - substituents)

Binding of β-ketoenoles to amyloid fibrils of insulin and lysozyme produces an increasing of specific fluorescent response (up to 60 times) with excitation and emission maxima at the range 408-458 and 486-552 nm, respectively; its intensity depends on the structure of substituents. Their quantum yields upon binding to insulin fibrils increase up to 0.19-0.40. The most amyloid-sensitive fluorescent response are observed for β-ketoenoles containing short hydroxyethylamino and methoxyethylamino tail groups. Lifetimes of the excited state of β-ketoenole dyes in complex with amyloid fibrils are characterized by two-component fluorescent decay. An average fluorescence decay timeare equals 1.03 ns for insulin fibrils and 1.16 ns for lysozyme fibrils.

In conclusion, we report β-ketoenoles as fluorescent molecules sensitive to amyloid fibrils formed by different proteins and propose them as probes for *in vitro* studies connected with amyloid-related diseases.

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CP MAS Kinetics Study in Glycine Powder Sample

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Nuclear Magnetic Resonance (NMR) is progressively marching into the field of crystallography. It opens the new possibilities to investigate complex systems like powder, confined, meso- and nano-structured materials [1-2].

$^{1}H\rightarrow^{13}C$ Cross Polarization (CP) kinetics upon Magic Angle Spinning (MAS) in glycine powder was studied in the present work. Even in this simple molecule, two distinct ^{13}C signals yield different CP kinetics (Fig. 1). Acquired curves were analyzed using well refined spin coupling models [1].

It was deduced, that these differences occur because of the distinctive neighboring proton properties in the nano-scales. Hence, used CP model has to be adjustable in order to obtain correct structural information.

NMR measurements were carried out at room temperature on Bruker AVANCE III HD spectrometer operating at 400 MHz proton resonance frequency. The MAS rate was 7 kHz.

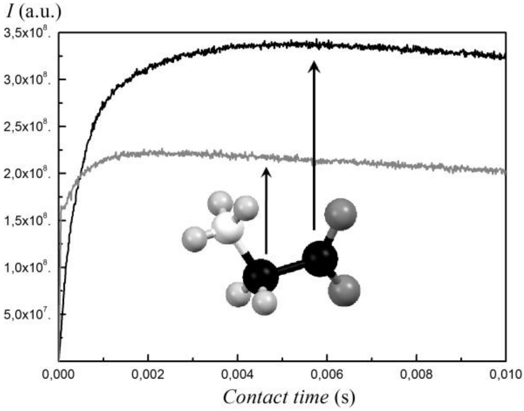

Fig. 1. $^{1}H\rightarrow^{13}C$ CPMAS kinetics curves for separate glycine peaks.

[1]. V. Klimavičius et al. CP MAS Kinetics Study of Ionic Liquids Confined in Mesoporous Silica: Convergence of Non-Classical and Classical Spin Coupling Models // Applied Magnetic Resonance. – 2017. DOI:10.1007/s00723-017-0891-z.

[2]. L. Dagys et al. Processing of CP MAS kinetics: Towards NMR crystallography for complex solids. // J. Chem. Phys.–2016. V. 145.– p. 114202 (9).

Capacitive Spectroscopy of Defects in Semiconductors with Impurity of Zirconium

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In recent years, monocrystalline silicon is the main material of microelectronics. For the monitored control parameters of the silicon are increasingly being used unconventional doping impurities [1-4], examples of such impurities are refractory elements. Typical representatives of these elements in the silicon atoms of hafnium, molybdenum, zirconium, etc.

Therefore, the aim of this work is to study the energy spectrum of defects in silicon, doped with one of these elements, zirconium introduced in the Si diffusion method. As the samples were used monocrystalline silicon n- and p-type conductivity with different resistivity.

Silicon doping with zirconium was carried out by diffusion method from the deposited layer of high purity Zr in the temperature range 1000÷1250 °C for 1÷50 hours. Cooling of the samples after the diffusion of Zr was carried out in various ways. As control was used the samples of n - and p-Si heat-treated at the same temperature and time as the introduction of Zr in Si.

The measurement results showed that in all samples n-Si after doping with zirconium to an increase in magnitude of the resistivity. In the samples p-Si of resistivity remains almost unchanged.

For the samples Si, diffusion-doped with Zirconium, as well as subjected to control heat treatment were measured DLTS spectra. Analysis of the DLTS spectra of samples n-Si <Zr> shows that the presence of Zr in Si leads to the formation of three deep levels with fixed ionization energies of E_C-0.22 eV, E_C-0.42 eV and E_V+0.30 eV, the dominant ones are the last two levels. Parallel measurements of the spectra of DLTS in the control treated samples of n-Si have shown that they have only a level with an ionization energy of E_C-0.22 eV, and its concentration is much higher than in the samples doped with zirconium.

Experiments with low-temperature treatments (LTT) showed that isothermal annealing in the temperature range of 100÷300^{0}C leads to reduction of the concentration of deep levels E_C-0.42 eV and E_V +0.30 eV, and an E_C-0.22 eV is stable to the effects of LTT. Preliminary measurements of the spectra of infrared absorption in samples Si<Zr> showed reduction in the concentration of optically active oxygen.

[1]. Milnes A. Impurities with deep levels in semiconductors. – M., Mir, 1977, 547c.

Determination of the Content of Heavy Metals and Organic Substances from Municipal Solid Waste Incineration Bottom Ash

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As an on-going concern in the management of waste more and more consideration is given to recycling and reuse of residues for construction purposes. The legislation for utilization is being tightened and the amount of municipal solid waste incineration (MSWI) bottom ash is rising. MSWI reduces the volume of waste approximately 90%, in mass- 70%. MSWI bottom ash may be important for building industry, however it content of heavy metals need a studying. Burning of garbage creates emission and residues. The particles with diameter ranging from 0 mm to 40 mm coming out with bottom's part of the plant's furnace consist of glass, ceramics, inorganic materials, different metals such as Fe, Cr, Cu, Al, Zn, Mo. Basic aim of the research consists of the detection of these substances and detection of the sizes. Using of X-Ray Spectroscopy allows determining of heavy metals content.Content of heavy metals is placed into a range of permissible concentration. With the help of atom absorption vibration spectroscopy, we found a number of organic aromatic molecules and do correction analysis. The results of this study is proposed to be used in the building industry for production of building blocks.

Light Sources Impact on Human Circadian Rhythms

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Nowadays, LED light sources are becoming wide use due to their energy efficiency, environmental compatibility and ample opportunities for the light field configuration [1,2]. Light has multifaceted impact on humans including their psychological and physiological state. Due to non-visual photoreceptors of the eye, human circadian rhythms are determined by light intensity, color temperature and short-wave part of the spectrum [3]. For this reason, LED lighting impact on human circadian rhythms is actively studied. In the research the impact of the white LED lighting and artificial light sources of different nature as well as standard light sources on human circadian rhythms was analyzed. Special A_{CV} factor denotes the "dose of blue light" affecting non-visual photoreceptors per one lumen. It was calculated for a number of lights sources from their spectral characteristics (Table 1). Obtained results demonstrate independence of A_{CV} factor values from the type of light sources with the similar correlated color temperatures (CCT). The "dose of blue light" increases almost linearly with the correlated color temperature increasing. For CCT of about 4000 K and 6000 K the A_{CV} factor is more than 1.4 and 2.0 times higher compared with the type A light source. Thus, it is very important to use the natural white light dynamic change throughout the day with natural and cold tones of the white light from the morning to afternoon and with warm tones in the evening.

Table 1. A_{CV} factor and CCT for different light source types.

Incandescent lamps	*CCT, K*	*2737*	*2833*	*3000*	
	A_{CV}, W/lm	0.51	0.54	0.6	
Standard sources	*CCT, K*	*2856(A)*	*4870(B)*		*6500(D65)*
	A_{CV}, W/lm	0.55	1.11		1.37
Luminescent lamps	*CCT, K*	*2428*	*3990*	*5956*	–
	A_{CV}, W/lm	0.30	0.71	1.10	–
LED lamps	*CCT, K*	*2731*	*4119*	*6004*	*6801*
	A_{CV}, W/lm	0.47	0.82	1.19	1.32

[1]. E.F. Schubert. Light-emitting diodes. // New York: Cambridge University Press. – 2008.
[2]. Z. Gotra et al. Energy efficient LED lighting systems. // Kyiv: PH «Avicena». – 2016.
[3]. M. Rea et al. The potential of outdoor lighting for stimulating the human circadian system // Sovremennaya Svetotechnika. – 2010. – p. 54 – 58.

AIE Based Coumarin Chromophores. Theoretical Study

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At present, a significant interest of researchers is directed to one of the photophysical phenomena associated with the aggregation of chromophores - aggregate-induced emission (AIE). In the AIE process, non-emissive luminogens are induced to emit by the aggregate formation. On the basis of experimental and theoretical studies, the main mechanisms which responsible for the AIE effect are proposed [1]. None of them, however, can be fully supported by the experimental data or applicable to all the reported AIE systems. In recent years Wang and co-workers report AIE active coumarin-based Schiff bases [2]. However, for molecules of the coumarin series which possess the properties of an AIE, none of the mechanisms cannot fully describe the features of fluorescent characteristics. To decipher AIE process, the first step is to learn emission quenching of single molecules of AIEgens by radiationless processes in the solution state. In this respect, we carried out theoretical calculations of the absorption spectra of the model series: coumarin, 3,4-benzocoumarin, 4,9-dioxapirene-5,10-dione (DPD). The quantum-chemical calculationsof the energy parametersof the modelcompounds were performed employing the program packageGAUSSIAN 03Wwithindensity functional theory(TD-DFT)B3LYP methodandbasis set6-31G(d). The position of energy levels electronic-excited states of model compounds and the energy gap between $S_{\pi\pi}$ and $T_{n\pi}$-levels with an increase in the size of the π-system was explored using the results of calculations. The influence of temperature on the spectral-luminescent properties of molecules is discussed. It was confirmed that the effect of temperature should be associated with a change in the length of the C=O fragment and, correspondingly, a change in the relative position of the energy levels of the lower electronic-excited states. The discussion of the possible mechanism of the AIE-coumarin molecules was based on the established basic regularity of the change in their spectral-luminescent properties, which is determined by the relative position and proximity of the energy levels of the lowest electron-excited states of different orbital and spin nature.

[1]. Ju Mei, Nelson L. C. Leung, Ryan T. K. Kwok, Jacky W. Y. Lam, Ben Zhong Tang. Aggregation-Induced Emission: Together We Shine, United We Soar // Chem. Rev. - 2015. – 115(21). – p. 11718-11940.

[2]. H. Xiao, K. Chen, D. Cui, N. Jiang, G. Yin, J. Wang, Wang R.Two. Novel Aggregation-Induced Emission Active Coumarin-Based Schiff Bases and Their Applications in Cell Imaging// New J. Chem. – 2014. – 38. – p. 2386−2393.

Investigation of Mechanisms of Potassium and Cesium-137 Uptake by Plants with Optical and Gamma Spectrometry in the Field under Water-Stressed conditions

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The mechanisms of potassium (K) and cesium (^{137}Cs) uptake by plants were studied using different plants. The investigations were performed at three experimental field sites within the 10 km Zone of the Chornobyl Nuclear Power Plant in 2012 and 2013. Plants seeds were sown, and plants and their corresponding soil solutions were sampled, several times during each growing season. Humidity of soils were determined for each of the selected soil sample. Soil solution was extracted by a centrifuge from every soil sample. The obtained soil solution was first filtered through filter paper with a pore diameter 1-3 μm, and then through a membrane filter with a pore diameter of 0,1 mkm. The concentration of ^{137}Cs in the samples was determined by a gamma-spectrometer with the semiconductor detector HPGe ORTEC GMX40P4-83-RB POPTOP sn.48-TN22465A. Potassium concentrations at the samples of soil solutions and at the samples of dissolved plants were measured by an optical method by atomic-absorbing spectrometer C-115-M1. Discrimination factor DF = $(^{137}\mathrm{Cs/K})_p/(^{137}\mathrm{Cs/K})_{ss}$ was estimated for each paired sample. Here, $(^{137}\mathrm{Cs/K})_p$ is the quotient of ^{137}CsandK concentrations in the plant and $(^{137}\mathrm{Cs/K})_{ss}$ is the same for the corresponding soil solution. It was observed that potassium and cesium entered plant roots, as a rule, through a complement of transporters with low selectivity when the concentration of dissolved potassium (C_K) in the soil solution was greater than 2 to 4 μg/cm^3. In this case the value of DF was near 1. However, when C_K was between 0.5 and 2 to 4 μg/cm^3, potassium also appeared to enter plant roots through highly-selective potassium transporters, whilst cesium entered roots only through the transporters with low selectivity. In this case the value of DF was much less than 1. When C_K was less than 0.5 μg/cm^3, cesium appeared to enter roots through a complement of transporters with greater selectivity for cesium than potassium. The value of DF in this case could exceed 1.

Spectrophotometric Monitoring of Converting Leuco Form of Indigo Carmine in Its Colored Form: Kinetics of Oxidation in Polymer Films with Different Oxygen Permeability

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Monitoring of oxygen concentration in various media is very important in medical, biomedical and environmental sciences, as well as in industrial processing, where oxygen is often involved as reactant or product. Technical and patent literature provide several examples of the optical sensors for oxygen the most common of which are sensors based on the quenching of luminescence of appropriate indicators [1,2]. Various methods for fluorescence sensing have been investigated [3]. Disadvantage of method based on fluorescent measurement is that the fluorescence intensity can vary due to changes of many parameters [4].

In this study we reported four types of polymer systems with different oxygen permeability, including poly(ethylene –co-vinyl alcohol) (EVOH), EVOH, modified with 7% of N,N’-bis(2,2,6,6-tetramethyl-4-piperidyl)-isophtalamide (Nylostab S-EED), EVOH, modified with 10% of Nylostab S-EED, and polyisoprene that have been investigated as carrier for leuco form of Indigo Carmine. An irreversible and visible color change from yellowish to blue caused by a chromogenic reaction involving the oxidation of leuco dye of Indigo Carmine by molecular oxygen has been investigated in polymer media. The relationship between the oxygen permeability of polymer films and the rate of observed color changes (absorbance maximum at 610 nm) has been studied. The choice of selected polymers allowed variations in the oxygen permeability from 2.8 $cm^3/m^2/day$ to 23.3 $cm^3/m^2/day$. The possibility to use prepared materials as absorption-based opto-chemical sensors for oxygen has been discussed.

[1]. Xu-dong Wang and Otto S. Wolfbeis. Optical methods for sensing and imaging oxygen: materials, spectroscopies and applications //Chem. Soc. Rev. –2014. – V. **43.** – p. 3666-3761.

[2]. N.Barashkov, I.Irgibayeva, T.Sakhno. Investigation of relationship between the rate of converting leuco form of Indigo Carmine in its colored form and oxygen permeability of polymer films // 253rd ACS National Meeting in San Francisco, California, April 2-6, 2017.

[3]. C. McDonagh, C.S. Burke, B.D. MacCraith. Optical chemical sensors // Chem. Rev. – 2008. – V. 108. – p. 400–422.

[4]. M.Y. Berezin, S. Achilefu. Fluorescence lifetime measurements and biological imaging, Chem. Rev. – 2010. – V. 110. – p. 2641–2684.

The Problem of Quality and Safety of Activated Carbon

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One of the reasons for non-compliance of medicines regulatory requirements GMP (Good Manufacturing Practice) - is microbiological contamination.

As a result of checking compliance with activated charcoal "Silkarbon" for the production of sterile drugs for compliance with regulatory documents found (Table 1) that microbiological purity (MKYA number UA/11425/01/01), it is responsible for the total number of aerobic microorganisms (TAMC), but is not responsible for the total number of yeast and mold fungi (ТУМС).

Table 1. The results verify that activated charcoal

Performance	Requirements Sun	Result
Microbiological purity:		
- total number of aerobic microorganisms (TAMC)	not more 10^3 CFU/g	responsible (500 CFU/g)
- the total number of yeast and mold fungi (TYMC)	not more 10^2 CFU/g	**does not meet the** (2575 CFU/g)

After analysing the proposed methods and devices for the antibacterial disinfection of such material, scientific and technical center of Poltava University of Economics and Trade experimental work conducted by irradiation of activated carbon particles during their free fall UV lamps, low pressure with a wavelength of 253.7 nm, which has bactericidal action and provides effective inactivation of microorganisms of various types [1].

The results of UV irradiation activated carbon showed a significant reduction in the overall degree of inactivation of yeast and mold fungi (TYMC). Depending on the dose amount of yeast and mold fungi is reduced by two orders of magnitude that satisfies the requirements of regulatory documents for microbiological analysis.

[1]. Semenov, A.A., Kozhushko, G.M. Bactericidal irradiators for ultraviolet disinfection of indoor air // European Applied Sciences. – 2013. – Vol. 1(13). – P. 226-228.

Features of Automation of Spectroellipsometric Measurements within Range of 1-4.9 eV

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The main purpose is to automate the process of ellipsometric measurements in wide spectral range in order to accelerate the measurement, and improve its accuracy minimizing the number of the possible errors that can be associated with the human factor. We proposed automation of spectroellipsometer to measure optical properties of sample surfaces by Beattie-Conn method. The experimental setup is shown in Fig. 1.

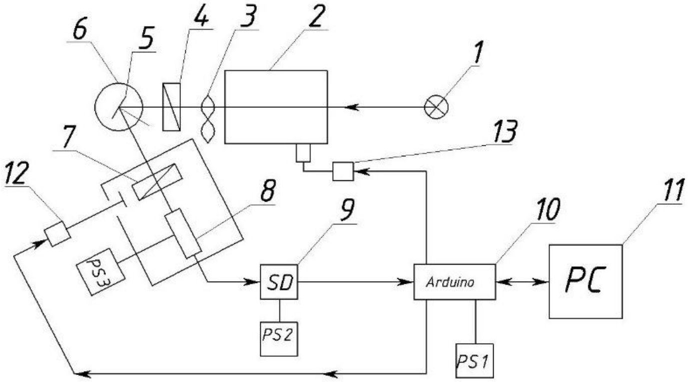

Fig. 1. The scheme of the device

The light from the source (1) passes through the optical system of the monochromator DMR-4 (2), modulator (3) (with constant frequency of modulation) and polarizer (4) (fixed azimuthal position) and then falls on the surface of the sample (5), which is fixed on moving table (6). Other reflection light beam passes through the rotatable analyzer (7) (at fixed azimuthal positions at 0°, 45°, and 90° of Beattie-Conn method) and reaches the photoelectronic multiplier (8) (the analyzer and photoelectronic multiplier are also rotatable around the vertical goniometer axis). Analogue signal from the photoelectronic multiplier is sent to lock-in amplifier (9), and the signal from lock-in amplifier (9) then reaches the controller (10) which provides the conversation of analog signal to digital one and data exchange with a PC (11). The measurements of light beam intensity are provided by different azimuths of the analyzer (7), which can be rotated by stepper motor (12).

The wavelength scanning is provided by rotation of the monochromator screw by stepper motor (13). The wavelength scanning range is from 0.24 to 1.2 μm. Software for signal processing is based on the object-oriented programming language C#. The program provides an opportunity to measure the intensity of light flux at fixed azimuths of analyzer namely α = 0°, 45°, -45°, 90° and -90°, and conduct an instrument calibration and self-diagnosis of the all electronic components of the automated spectroellipsometer. It is necessary to install the sample on the table then to calibrate the azimuths of the analyzer in condition that the reflected light reaches photoelectric multiplier, in such manner the azimuthal positions of analyzer and polarizer by software are calibrated. Then the range of wavelength is chosen in order to input them to the program for an installation of the monochromator screw at the start position of the selected spectral range. Then one press is START button and the process of measurement should be started. For one of the wavelengths the intensities of light at the fixed azimuths of the analyzer namely 0°, 45°, -45°, 90° and -90°, are measured. The measurements must be made at every 45° azimuth of the analyzer. The values of a voltage at every position of the analyzer is digitized in the controller and passed to PC for the next processing in the software. For the taken intensity values tg(ψ) and cos(Δ) were calculated due to Beattie-Conn method and then the graphs of tg(ψ) and cos(Δ) were built in dependence on the wavelengths. The automation of the spectroellipsometric device allows to reduce time of measurements of ellipsometry parameters tg(ψ) and cos(Δ), and now the time of the measurement at each wavelength is of about 8-10 seconds.

Spectroscopy of Molecules Adsorption on the Surface of Piezoelectric Crystal

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During mechanical deformation in piezoelectric an electrical polarization occurs, which brings to radiation of electromagnetic waves. This phenomenon may be used for investigation of adsorption processes on the surface of piezoelectric. Hamiltonian formalism and apparatus of temporal retarded Green functions is used for description of studied processes.

If motion of charge, during adsorption process, is induced by the electromagnetic field of crystal, then in frames of the linear response theory, the quantum-statistical average value of current density may be expressed by the intensity of electromagnetic field of crystal and temporal retarded Green function based on operators of current density and polarization, which in turn may be expressed through Green function of polarization operators, if the relation between polarization and current density will be considered.

As a result, a correlation for a Fourier component of current density with the Green function of polarization operators, which may be expressed through the complex dielectric permeability of a medium, may be obtained. Accordingly, an expression of the temporal Fourier component of the vector-potential in the long-wave approximation will be obtained, caused by adsorption process.

The intensity of electromagnetic radiation will be determined by the structure of the crystal and by the size of deformation, which may change as a function of time. As a result, because deformation changes in time, the intensity of electromagnetic radiation also changes in time, so, that will allow observation of frequency spectrum and the value of external action.

Spectrophotometric Control Oxidation-Reduction-Potential (ORP) of Water During Its Activation

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One of the characteristics of water containing dissolved molecular hydrogen (such as ionized water) is that it exhibits a negative oxidation-reduction potential (O.R.P.). Chemical reactions occurring in an aqueous solution are called redox reactions. The ORP measures the capacity of a solution to either release or accept electrons from chemical reactions. The ORP value, much like pH, is important for determining water quality and for water treatment processes, the perspective for modern medicine. The disease occurs when cells ORP deviate from the norm (when the cells lose their negative potential). Activated in any way water becomes, for example, a negative potential, easily absorbed by the body and restores the negative potential of cells lost during disease.Non-contact activation methods of biological fluids without changing their chemical composition are remarkable [1]. The design we used as activator is the plastic bag inside with powdered magnesium and some water placed inside. The package sealed and immersed in the test liquid (water). During the interaction of magnesium with water inside the package generated hydrogen that diffuses through the walls outside of the package, thus, saturating with hydrogen water surrounding the package. As a result, ORP of water changes towards negative and can reach sizes "-" 600 mV.

Our proposed method provides greater speed, allows to visualize the distribution of ORP in the volume liquid medium and its rapid changes.

[1]. Prilutsky VI, Bakhir VM Electrochemically activated water: Abnormal properties, the mechanism of biological action. - M .; VNIIIMT of JSC NPO "Ekran". 1997, 228 pp. Http://www.ikar.udm.ru/sb/sb10-1.htm).

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Last Minute Abstracts

Spectral and quantum mechanical study of iso-quinolinium-carbethoxy-cyano-methylid

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Iso-quinolinium-carbethoxy-cyano-methylid is a dipolar molecule with one electronic visible band due to an intramolecular charge transfer from carbanion toward heterocycle. The solvatochromic study has been realized using the position of this electronic band in the wavenumber scale in different diluted solutions. The quantum chemical results, obtained based on Spartan'14 programs, were correlated with those obtained by solvatochromism.

The dipole moment in the excited state of iso-quinolinium-carbethoxy-cyano-methyl was estimated based on this study.

Synthesis and spectral analysis of a new antitumor compounds with benzimidazole structure

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Amidic compounds, derivatives of the 5-nitro-benzimidazolyl-2-mercapto-acetic acid were obtained in order to get new cytostatic substances. Two azotyperitic derivatives were obtained by the grafting of the di-(β-chloroethyl)-amine group on molecules of two of the amidic compounds.

The IR spectra were registered which confirmed the structure of the new compounds.

A spectrophotometric method using for evaluation human serum MCP-1/CCL2 levels in type 2 diabetic subjects

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Type 2 diabetes mellitus (T2DM) and obesity are major risk factors for cardiovascular disease. Monocyte chemoattractant protein-1 (MCP-1) is the first discovered and most studied chemokine, and a lot of studies on its role in the etiologies of obesity- and diabetes-related diseases have increased exponentially during the past years. The enzyme-linked Immunosorbent Assay (ELISA) is the gold standard clinical diagnostic tool for the detection and quantification of protein biomarkers.

The highlights of this paper include the evaluation of MCP-1 levels using enzyme-linked immunosorbent assay. The method applies absorption spectrophotometry to measure the absorbance (optical density) of the sample using a monochromatic light source and optical sensor. We examined three groups: patients with T2DM, T2DM and obesity and healthy volunteers group. Fasting blood samples were collected from each. We designed the study for comparisons between the mentioned groups regarding blood serum MCP-1/CCL2. Thus we also determined glycemia and the blood levels of the following: cholesterol, low-density lipoprotein cholesterol, and triglycerides. Blood serum MCP-1/CCL2 was measured using a commercially available ELISA kit. Compared to the healthy control group MCP-1/CCL2 was elevated in both study groups (T2DM, T2DM and obesity). Moreover, levels of serum glucose, MCP-1/CCL2 and lipid abnormalities were the highest in the T2DM+obesity group. We used the system for MCP1/CCL2 ELISA detection in huam serum. The device performs automated analysis of the results and presents absorbance values and diagnostic test results. The present work brings evidence that patients with established T2DM have a different cytokine profile compared to healthy controls and this could indicate changes in the immune function in T2DM patients.

Scattering of Ginzburg-Frank and Cherenkov Types under Self-focusing of Nanosecond Laser Pulse in Liquids

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The report is devoted to investigation of dynamics of nonlinear optical processes (self-focusing, self-phase modulation, stimulated Raman scattering) in Kerr-liquids (toluene, xylene, benzene etc.) under nanosecond laser pulse excitation.

The phase self-modulation of nanosecond laser pulses under the quasi-stationary self-focusing in the Kerr liquid is studied. Calculations of the additional phase delay, the instantaneous frequency and the pulse spectrum are carried out. The results of calculations and the experimental data prove the existence of the transition Ginzburg-Frank effect, which promotes the appearance of new spectral components at the medium boundary, when the focal area crosses the exit boundary of the medium. The spectral components, which arise owing to this effect, have the Stokes shift up to hundreds of inverse centimeters with respect to the exciting radiation frequency. The temporal and energy characteristics of the radiation that is generated as a result of the transition effect are specified.

Under the transition effect the maximum frequency shift of laser radiation appears, when focal point of self-focusing intersects exit boundary of the medium and phase delay before and after the focal point is uncompensated.

The mutual impact of self-focusing focal point velocity and self-phase modulation on the frequency-angular spectra of parametric SRS components is identified. The generation of extended SRS anti-Stokes frequency-angular bands is explained. When the velocity of self-focusing focal point matches the phase velocity of non-linear polarization at anti-Stokes Raman frequency and the phase velocity of the scattered axial radiation, the most intense frequency-angular bands appear, which are described by the equations typical to Cherenkov radiation. In particular, under excitation with nanosecond laser pulses in toluene such bands reach a length of about 200 cm^{-1} against the Raman anti-Stokes frequency to the Stokes side. This is result of superluminal speed of the focal point movement.

In both cases the new different frequency of radiation are result of temporary instability and self-phase modulation under extremal speed of the focal point movement.

Explanation of Stimulated Raman Scattering Indicatrix Asymmetry

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According to Placzek's theory, the cross-section of Raman scattering is the same in both forward and backward directions along the exciting laser beam. Completely different, in case of stimulated Raman scattering Stokes component the asymmetry is essential in almost all experimental conditions. Intensity of the forward stimulated Raman scattering first Stokes component is usually much higher than the intensity of the backward scattering, which propagates in the opposite direction with respect to the exciting laser beam. The nature of stimulated Raman scattering indicatrix asymmetry is still controversial.

The report provides experimental and theoretical results of stimulated Raman scattering indicatrix asymmetry study of Stokes component. Temporal experimental data and the theoretical description for asymmetry of the SRS Stokes component indicatrix under the Stokes/anti-Stokes parametric process are presented.

The competition between forward and backward scattering processes is important. Theoretical results demonstrate that asymmetry is caused by influence of Stokes/anti-Stokes parametric processes. Stokes/anti-Stokes parametric process provides additional photons to the forward Stokes component. This excess of photons compared to a backward Stokes component increases due to combinational mechanism of stimulated scattering during further propagation of waves along the medium. Thus, under competition of forward and backward Stokes components generation, the process of forward stimulated Raman scattering takes significant advantage.

Satisfactory matching between theoretical calculations and experimental results for benzene under excitation by laser pulses with duration 25 ns and wavelength 694.3 nm is obtained.

The calculated logarithm of the scattering asymmetry coefficient by intensity reaches value of ~1.6 at maximal laser radiation intensities. Experimental values of the asymmetry coefficient logarithm by energy are much higher and reach ~2.3 in similar conditions.

Differences of experimental and theoretical results might have appeared due to neglecting of radiation intensity change during the laser pulse. However, the more important is presence of self-phase modulation, despite the fact that benzene does not reveal distinct self-focusing properties.

Spectroscopic Features of Raman Gain Profile in Singlemode Fibers Based on Silica Glasses

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The Raman gain profile is key parameter for design both highly efficient fiber Raman lasers (FRL) and fiber Raman amplifiers (FRA) with working bandwidth up to 13 THz. Despite the Raman gain can be obtained using practically arbitrary type of silica fiber but its gain coefficient is strongly depends on many fiber parameters. For example Raman gain maxima in widespread silica fibers at approximately 440 cm^{-1} (it is equal to 13 THz of Stokes shift) are varied from 0.4 $(W \cdot km)^{-1}$ in pure silica fiber to 6.3 $(W \cdot km)^{-1}$ in highly GeO_2 doped silica fiber. In addition both Raman gain profiles are very complicated and its forms are significantly differed one from other within practically meaning Stokes shift band from 20 cm^{-1} to 1000 cm^{-1}.

The Raman gain profile can be clearly extracted from the experimental Raman spectrum as its temperature independent part. We propose to obtain the Raman gain profile in analytic form using multimode spectral decomposition in the predefined Stokes frequency region. Such spectroscopic problem is highly complicated in every optical fiber case and their general solutions have not been obtained yet. However, earlier in most cases we were able to find the special solution of this problem, particularly in the foremost TiO_2 doped fiber [1, 2]. It is resulted the Raman gain profile in a convenient analytical form that significantly simplifies the next mathematical modeling of all Raman devices.

[1]. G.S. Felinskyi, I.V. Serdeha, and V.I. Grygoruk. TiO_2-doped Singlemode Fiber as Active Medium for Raman Lasers / *in proc*. Int. Symp. on Advanced Material Research, ISAMR'2017, Seoul, Korea, March, 17 -19, 2017, p.109.

[2]. G.S. Felinskyi, I.M. Kudin, I.V. Serdeha. Lasing Band and Raman Gain Threshold in TiO_2 doped Single-mode Fiber. / *in Proc*. of the 2017 IEEE 37th Int. Conf. on Electronics and Nanotechnology (ELNANO), April 18-20, 2017, Kyiv, Ukraine, p.108-111.

Polar metal-formate frameworks templated with 1,2-diaminoethane-water assemblies showing ferromagnetic and ferroelectric properties

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A set of five novel formate frameworks templated with the assemblies comprising diprotonated 1,2-diaminoethane (DAE) and water molecule of the formula: $[NH_3(CH_2)_2NH_3]M_2(HCOO)_6{\cdot}H_2O$, where M = Mg, Mn, Co, Ni, Zn, has been synthesized. Four compounds crystallize in polar *R*3 and one - in chiral $P6_322$ space group (Ni-analogue) at room temperature. The polyammonium-water assemblies, mutually joined by hydrogen bonds, fill the cavities of the frameworks and are disordered in the three latter compounds. Additional disorder is found in Ni-sample since the DAE^{2+}-H_2O couple is placed in the special position of 6_3 screw axis. The IR spectroscopy provides the evidence of proton dynamic disorder within the assemblies, which turns into a static one at low temperatures.

The crystals preserve their arrangement up to approximately 370 K as shown by the differential calorimetric measurements and the temperature-dependent IR spectroscopy. The ferroelectric nature of a representative of the family – DAEMgF at room temperature has been confirmed by pyroelectric measurements. It has been found that the spontaneous polarization may be changed by an external electric field. The magnetic studies reveal a weak ferromagnetic behavior within 8.5-35 K for magnetically active ions: Mn, Co and Ni.

†Electronic supplementary information (ESI) will be available in the online version of the manuscript.

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