XXII Galyna Puchkovska
International School-Seminar

Spectroscopy of Molecules and Crystals

Book of Abstracts

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Institute of Physics of National Academy of Sciencies of Ukraine
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The Book contains abstracts of reports presented at XXII Galyna Puchkovska International School-Seminar “Spectroscopy of Molecules and Crystals” (September 27 – October 4, 2015, Chynadiyovo, Zakarpattia, Ukraine). The abstracts cover recent advances in theoretical and experimental spectroscopy of crystalline and amorphous solids, liquids and gases, liquid crystals, 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. Abstracts, submitted according to ISSSMC rules, are published as received from the authors. The Book of Abstracts is approved for publication by the Scientific Council of the Institute of Physics of the National Academy of Sciences of Ukraine (Protocol No. 9 of 31.08.2015).

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В збірнику представлені тези доповідей XXII Міжнародної Школи-семінару імені Галини Пучковської “Спектроскопія молекул і кристалів” (27 вересня – 4 жовтня, 2015, Чинадійово, Закарпаття, Україна). В тезах викладено нові результати досліджень з основних напрямків сучасної теоретичної і експериментальної спектроскопії неметалічних кристалів, аморфних речовин, газів, рідин, рідких кристалів, полімерів, 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. Тези, надані у відповідності до правил ISSSMC, надруковано в авторському поданні. Книга Тез рекомендована до друку Вченою радою Інституту фізики НАН України (Протокол № 9 від 31.08.2015).

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Dear participants of the XXII ISSSMC,

On behalf of the Organizing Committee, I invite you to take active part in this international scientific event.

To our regret, XXII School-Seminar will be held not at our favorite Centre of recreation and tourism of Taras Shevchenko National University of Kyiv in Beregove, Crimea. I believe this is temporary. This year we propose you another beautiful Ukrainian place – Chynadiyovo in picturesque Zakarpattia.

Well-known scientists and permanent participants of ISSSMC, Professor Longin Lisetski and Professor Oleksandr Slobodyanyuk have written forewords for this Book of Abstracts.

Chair of International Program committee,
Professor Valeriy Pogorelov

During the last decade, we got accustomed to the Black Sea coast in Beregove, where scientists studying spectroscopy of molecules and crystals were meeting each other in the early autumn of each odd year. Rather specific landscapes of Western Crimea, with poor vegetation and gloomy beaches, did not prevent us from falling in love with that modest but enchanting corner of our land. Unfortunately, well-known tragic events in our country separated us from our familiar meeting place. However, there is nothing so bad as not to be good for something – and now we are going to gather in a much more picturesque place, with beautiful countryside, historical monuments, and wine cellars nearby. So, welcome to Chynadiyovo!

Chynadiyovo has been known since 1214 as a settlement of medieval Kyiv Rus’ (the present-day Ukraine). Historical annals clearly state that in 1247 Chynadiyovo belonged to Prince Rostyslav Mykhailovych – a grandson of Prince Roman Mstyslavych, i.e., a nephew of Danylo Halytskyi – the famous ruler of Halychyna-Volyn’ princedom, who was crowned as King of Rus’ in 1254. Later, Rostyslav Mykhailovych became a son-in-law of Hungarian King Bela the Fourth, and these lands gradually fell under influence of Hungary. During its long history, Chynadiyovo knew many feudal rulers. After defeat of the so-called Rákóczi's War of Independence (1711), Charles the Sixth, Emperor of the Holy Roman Empire from the Habsburg House, granted Chynadiyovo as a present to Lothar Franz von Schönborn, Archbishop-Elector of Mainz. The main architectural attraction of Chynadiyovo, the Schönborn Palace, is a memorial of those times. Before 1944, Chynadiyovo was known under its Hungarian name – Szentmiklós, which means “St.Nicholas”.

One can see that Chynadiyovo has been going, via multiple stages, along a long circular (or helical) path – from a Ukrainian village in Kyiv Rus’ to a village in modern independent Ukraine. In a similar way, our School-Seminar, which was first launched in Uzhgorod (in Zakarpattia Oblast) in 1973, has returned to its initial geographical surroundings.

Chynadiyovo is located close to the officially recognized geographical center of Europe, which is considered to be also in Zakarpattia Oblast.

Looking at the map, one can notice that Chynadiyovo is nearly equidistant from the borders of several neighboring countries – Romania, Hungary, Slovakia… In the same way, the scientific scope of our School-Seminar is a natural meeting point of multiple fields and directions of modern science.

Some words about the scope of our meeting. The word “spectroscopy” recalls a vast multitude of different kinds of spectra. Absorption, transmission, luminescence, selective reflection, UV, IR, X-ray, Raman, Fourier, NMR, SEIRA, SERS, Mössbauer, and maybe even NEXAFS – endless variety and infinite prospects for expansion and development. As for “molecules and crystals” – could anybody name any material object not composed of molecules and having no signs of crystalline structure? If you think about solutions and melts of some inorganic salts – but they also can be studied by spectroscopy; and even specialists in dark matter or Higgs bosons sometimes require scintillation spectra to detect their particles. Therefore, our School-Seminar is definitely a meeting of scientists dealing with the most advanced fields of modern scientific research.

Many of us remember that “in good old days” there were many similar conferences and meetings organized in parallel to our School-Seminars. Non-linear optics, liquid crystals, organic semiconductors, conformations and structure of molecules…. Most of them have been gradually fading out, while our School-Seminar seems to go marching on. One can ask – why? I would take the liberty of giving an answer. There is a wide known concept that everything in our world goes successfully when it is inspired by the Saint Spirit. In our case, this inspiration from Heavens comes via the soul of Galina Puchkovska – the founder and perennial organizer of our School-Seminars. As most of the old-time participants of our School-Seminars (and many, many others), I will always remember several occasions in my life when help and advice of Galina Oleksandrivna had a decisive impact on my scientific fortune. Moreover, we are sure that Galina Puchkovska International School-Seminar “Spectroscopy of Molecules and Crystals” will be a success – both this year and on many occasions in future.

Professor Longin Lisetski,
ISSSMC International Program committee

Know the invisible from the visible
Hryhorii Skovoroda, Ukrainian philosopher, 1722-1794

People tend to notice the coincidence of numbers, dates, places and other attributes related to the different events, and some people even give to these coincidences symbolic significance. The XXII International School-Seminar “Spectroscopy of Molecules and Crystals” (ISSSMC) is no exception.

For physicists, particularly those dealing with optical radiation and its interaction with matter, cannot stay out of sight of the fact the UN General Assembly 68th Session proclaimed 2015 as the International Year of Light and Light-based Technologies (IYL 2015). The UN has recognized the importance of raising global awareness about how light-based technologies promote sustainable development and provide solutions to global challenges in energy, education, agriculture and health. Light plays a vital role in our daily life and is an imperative crosscutting discipline of science in the 21st century. It has revolutionized medicine, opened up international communication via the Internet, and continues to be central to linking cultural, economic and political aspects of the global society.

Contribution of the optical spectroscopy as a leading Light-based Technology to the development of science and humanity is priceless. Without optical spectroscopy there would not be, on the one hand, Balmer series, Rydberg-Ritz combination principle and Niels Bohr's atom, and, on the other hand, Planck formula, quantum mechanics, and quantum electrodynamics, which create basis of Standard Model of particle physics and Standard cosmological (Big Bang) model. Without optical spectroscopy hard to imagine the possibility of creating the material base of modern global information society: semiconductor lasers, supertransparent optical fibers, CCD cameras etc. The Nobel Prizes in Physics 2000 and 2009 were awarded "for basic work on information and communication technology" and "for groundbreaking achievements concerning the transmission of light in fibers for optical communication and for the invention of an imaging semiconductor circuit - the CCD sensor”.

The first SSSMC was organized in 1973 (43 years ago) in Uzhhorod (43 km in a straight line from the venue of the XXII ISSSMC) by "the young and the restless" female team headed by Galyna Puchkovska and strongly supported by the leadership of the Institute of Physics, Ukrainian Academy of Sciences. Maybe, that's why from the very beginning the SSSMC did not follow a solid academic canon but made history thanks to the such hallmarks as extremely broad range of participants from students to academicians combined with unprecedentedly democratic style of participants' communication, regardless of their status and irrespective of the place: hall of plenary sessions, poster session, dining room, lobby, sightseeing bus or even beach. A youth had unique possibility to communicate with any participant including academicians A.F. Pryhot'ko, S.I. Pekar, A.S. Davydov, M.T. Shpak and many others. Today, some former students have become academics and themselves give lectures in ISSSMC to future generations of students. In addition, it should be noted that SSSMC from the outset had essentially international character, although international sign was added to the title only in 1981, on the eve of independence of the republics of the former Soviet Union.

Now the last but not the least. For people born and raised in the Soviet Union the number of ISSSMC in his Roman numerals is associated with designation of Party Congresses. In particular, the XXII Party Congress of 1961 proclaimed, "that the current generation of Soviet people will live under communism." However, it occurred the XXVIII Congress was the last Congress of the CPSU just before the collapse of the Soviet Union. I believe that the number of ISSSMCs will inevitably exceed the number of Communist congresses because the real science is incompatible with the dogmas and must respond to the real needs of humanity. Moreover, optical spectroscopy as an important Light-based Technology will always be in demand and will soon have to be numbered with Arabic numerals as more compact.

Nevertheless, today let's keep trying to know the invisible from the visible.

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Lectures

Structure, spectroscopy and features of selected flavonoids and related compounds

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Numerous naturally occurring and synthetic compounds belonging to the group of flavonoids are currently a subject of a growing interest. This is due to their distinctive biological activity and the role they play in plant growth, human diet and healthcare. The compounds investigated by us belong to the subgroups of flavonols, diflavonols, coumarins and chalcones. Their structure comprises heterocyclic, carbonyl and hydroxyl oxygen atoms, which are involved in various inter- and intramolecular interactions in the crystalline solid and liquid phases.

The crystal structure of the selected compounds was determined using X-ray crystallography and interactions were identified and investigated using various crystallographic and computational methods and programs. It was revealed that various specific (mostly H-bonding) interactions are responsible for mutual arrangement of molecules and unique architecture of the compounds in the crystalline solid phase. Another issue that we investigated was electronic absorption and emission spectroscopy of the compounds in various liquid environments and wide range of pH. It was revealed that the compounds are very sensitive to polarity and donor-acceptor ability, as well as acidity–basicity of a medium. These features are a consequence of the ability of the compounds to undergo protonation/deprotonation, as well as their involvement in various types of interactions with the surrounding molecules. Knowledge of these features opens up possibilities for the prospective use of the compounds as indicators of properties of liquid environments. Also, the compounds appear to be very convenient models for investing basic physicochemical features of multifunctional organic compounds containing oxygen atoms.

The presentation will touch on issues discussed in several recently published papers, among others mentioned below [1-4].

Study supported by Polish State Funds for Scientific Research (530-8220-D493-14).

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Photophysics and spectroscopy of novel inorganic carbon materials

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Small brightly fluorescent carbon nanoparticles containing elements of graphene, graphene oxide, diamond and unorganized structures (C-dots) have emerged as a new class of materials important for optoelectronic, sensing and imaging applications. We analyze comparatively the properties of these diverse carbon nanomaterials obtained by different methods. The mechanisms of their light absorption and photoluminescence emission are still an open debate among researchers. Because of the variety of C-dots, it is highly important to summarize the emission mechanism for these kinds of carbon materials; doing so we will be able to guide the development of effective synthesis routes and novel applications.

This presentation will focus on the photoluminescence mechanism of C-dots. We compare three types of fluorescent C-dots: graphene quantum dots (GQDs), carbon nanodots (CNDs), and polymer dots (PDs) and analyze four reasonable mechanisms of their emission: the quantum confinement effect or conjugated π-domains, which are determined by the carbon core; the surface state, which is determined by hybridization of the carbon backbone and the connected chemical groups; the molecule state, which is determined solely by the fluorescent molecules connected on the surface or interior of the CDs; and the crosslink-enhanced emission (CEE) effect. Though these mechanisms are presently not firmly established, the arguments are presented for their common origin. Our own results obtained by single-molecular studies and time-resolved spectroscopy shed light on these mechanisms.

Regarding present and potential applications, we provide critical comparison with the other types of fluorescence reporters, such as organic dyes and semiconductor quantum dots. The possibilities for design on their basis of multifunctional nanocomposites on a broader scale of optoelectronic and biological imaging applications are outlined.

Surface enhanced spectroscopy: effects, mechanisms, application

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Effect of surface enhancement of optical signal from molecules located near rough metal surface or metallic particles are known from the 70 years of last century. Phenomenological theory of this effect was created by V. Kocobukin [1] and consists of least 2 main mechanisms, electromagnetic mechanism (EM) - an increase of the electromagnetic field near rough metal surface, and chemical mechanism (CM) - an increase of the dipole transition moment of the adsorbed molecules [1]. Now we know different realization of surface enhanced spectroscopy, SEIRA (surface enhanced infrared absorption spectroscopy), SERS (surface enhanced Raman scattering), SEF (surface enhanced fluorescence), SECARS (surface enhanced Coherent anti-Stockes Raman Scattering), SFG (Sum-Freguensy Generation) etc.

The first paper devoted to study of DNA from cancer cells on rough gold surface was published by scientists from Institute of Physics NASU, Kyiv, Ukraine in 2001 [2] that gave a possibility to reveal a conformation peculiarities of DNA from cancer cells with high sensitivity and then these data were included in European tables on vibrational spectra of biological molecules.

During last decade we have been developing methods of surface enhanced spectroscopy (SES), namely, surface enhanced infrared spectroscopy (SEIRA), surface enhanced Raman scattering (SERS), surface enhanced luminescence (SEL), surface enhanced coherent anti-Stokes Raman scattering (SECARS) and their application. The phenomenon of SES is a sensitive tool for probing materials of small amount as well as molecules with low luminescence yield. Application of substrates of non-metallic nature, namely (carbon nanotubes, graphene, etc.) as well different semiconductor in the visible and IR region with negative real part of dielectric permeability for SES is demonstrated also.

Here we discuss possible mechanisms, as well as advantages and disadvantages of SES for identifications and analysis of biomolecules and their conformations, nanoparticles, stains and its origin.

We thank to Faemcar Project FP7-PEOPLE-2012-IRSES and Poland-Ukrainian Project 2015-2017 for financial support.

[1] V.A. Kosobukin. DAN SSSR, Ser.Fiz. **49(6)** (1985)1111.
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Thermoluminescence spectroscopy study of disordered conjugated polymer films: what can we learn from these measurements?

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This work provides an overview of thermally-stimulated luminescence (TSL) studies performed in conjugated polymer films and discusses in details physical process responsible for the TSL phenomenon in these materials. A broad range of organic photoconducting pi- and sigma- conjugated polymers was investigated including technologically important optoelectronic polymers as substituted poly(paraphenylene), different substituted poly(phenylene-vinylenes), poly(thiophenes), poly(fluorenes), poly(silylenes), etc. The obtained results are interpreted in terms of the thermally assisted hopping model of TSL we have developed and analysis of the TSL data allows evaluation of very important material parameters of these organic materials.

Topics covered in this paper: (i) excitonic and charged states in conjugated polymers; (ii) origin of energetic and positional disorder in these materials; (iii) basics of mechanisms of charge carrier photogeneration and charge transport in conjugated polymers; (iv) Anderson localization, hopping transport concepts and Miller-Abrahams jump rate; (v) basics of Gaussian disorder formalism with application to conjugated polymers; (vi) TSL experimental method and its application for charge trapping study and evaluation of the density-of-state distribution in conjugated polymers; (vii) our theoretical model of TSL and thermally-stimulated current (TSC); and (viii) critical comparison of different TSL models proposed in literature and fallacies underlying them. This lecture will introduce these topics and connect them to the current state-of-the-art.

Finally, I will show the application of TSL for evaluation of the energy splitting separating the singlet and triplet states of the interchain polaron pairs, which are the precursors of the electroluminescent species in conjugated polymers.

UV-induced effects in liquid crystalline systems

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A review is presented of various effects that can be induced in liquid crystalline (LC) systems containing photosensitive components, i.e., substances with molecules subject to structural changes under UV irradiation.

As the most known example, azoxy nematics undergoing *trans-cis-trans* isomerisation are considered. Of special interest are helically twisted cholesterics with such components, yielding ample possibilities in different fields - from fundamental aspects of the helical twisting theory to reversible tuning of lasing frequency in the distributed feedback dye lasers.

Combining chirality and photosensitivity in one and the same substance, one can realize various effects related to photoinduced changes in cholesteric textures, which are promising for application in optoelectronic devices.

An interesting possibility is offered by photosensitive substances of biological origin, which can be used, in parallel studies, as components of cholesteric mixtures (opening the prospects of bioequivalent radiation detectors) and as membranotropic agents (dopants) in multibilayer structures of hydrated phospholipids. The obtained experimental data serve as a basis for bridging the gap between thermotropic and lyotropic liquid crystal systems.

Special attention is paid to recent data on LC systems with dispersed carbon nanotubes (CNT) and other nanoparticles. With LC host including photosensitive components, CNTs can substantially affect the photoinduced processes. Moreover, there are prospects of essentially new effects based on joint application of electric field and UV radiation – a sort of “LC photoelectrooptics”. In particular, certain unusual properties are noted for mixtures of nematics with opposite signs of dielectric anisotropy (e.g., azoxy and cyanobiphenyls).

Great names in photophysics and spectroscopy: Sergey Vavilov and Aleksander Jabłoński

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Interaction of light with matter attracted many bright minds through the centuries. But only in the middle of XX century photophysics and spectroscopy has developed into powerful branch of research and found numerous important applications. Among many scientists who contributed to this tremendous progress of human knowledge the names of Sergey Vavilov and Aleksander Jabłoński shine especially bright. The famous Jabłoński diagram is no less important to physicists as the periodic table of elements for chemists, and every textbook of physics contains the explanation of Vavilov law. They were of almost the same age; both lived a long life reaching high level of recognition in research community. But they were quite different personalities, and their fate was different.

Russian Sergey Vavilov was born in Moscow in 1981 in the family of rich businessmen. His elder brother Nikolai became famous biologist (died in Soviet jail in 1943), but Sergey chose physics. He graduated from Moscow university in 1914 and soon was recruited to Russian army to serve indifferent engineering military units. After the war and Russian revolution, he started carrier as researcher and educator in physics. His impact on photophysics was fundamental. It was him who introduced the term quantum yield of fluorescence and formulated a fundamental law on independence of quantum yield on excitation wavelength.

Ukrainian Aleksander Jabłoński was born in 1898 in Voskresenka close to Kharkiv. He studied physics in Kharkiv University, and, when the First World War started he was recruited to Russian army. Soon Russian revolution began and when Poland declared independence he joined the Polish army and in 1919-1920 he fought for Poland against the aggression of Russian Red army. Thus, two great physicists could meet fighting against each other in a military battle. After the war, Aleksander remained in Poland that became his home country throughout his life. For some time, he studied music, but finally he chose physics. Remarkably, his PhD thesis had the title "*On the influence of the change of the wavelength of excitation light on the fluorescence spectra*", just in the same line as the Vavilov law. Jabłoński was a pioneer of molecular photophysics, creating the concept of the "luminescent centre". He developed the theory of concentrational quenching and depolarization of photoluminescence. His famous Jabłoński diagram was proposed 1933. It allowed illustrating schematically on an energy scale the processes of absorption and emission of light in the form of emissive and non-emissive transitions between electronic and electronic-vibrational energy levels.

It is still unknown if these two scientists ever met in person, since Soviet Union for many years was a closed scientific community. Probably only after the war, when Poland became a part of Socialist block. But no doubt, throughout decades they studied precisely the publications of each other as well as all physical community throughout the World analyzed and discussed their tremendous achievements.

The Nature of the Surface Chemical Bond Through X-Ray Spectroscopy and DFT

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When molecules bind to a substrate, the electronic structure, which was optimal for the internal bonds in the molecule, must be rearranged to allow bonding also to the surface. How this rehybridization occurs depends on the type of bond to be formed and the molecule and its available excited states. In the talk I will discuss six prototypical cases: (1) atomic radical adsorption and the *d*-band model [1] (C, N, O); (2) unsaturated π-systems (CO, N_2); (3) unsaturated hydrocarbons (acetylene, ethylene, benzene); (4) lone-pair bonding (H_2O); (5) physisorption (methane, *n*-octane); (6) hydrogen-bonding (water and ice). The material is based on x-ray spectroscopic, XAS and XES, studies combined with density functional calculations [2,3]. The scope is to give simple, intuitive pictures with which to analyze chemical bond formation. If time permits I will discuss our recent applications of this approach using the LCLS (Linac Coherent Light Source) free-electron x-ray laser to investigate CO desorption [4] and oxidation [5] on Ru(0001).

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Structure of Water in Condensed Phase

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Recently we can see high interest to the most important liquid on our planet – water. Different reviews and original papers on this theme regularly appear [1-3]. It is easy to find numerous systematics (the references) of the works, devoted to experimental and theoretical investigations of the unusual properties of water. Apparently, the Conference “Water – the most anomalous liquid” (Nordic Institute for the Theoretical Physics, Stockholm University, 13 October – 7 November 2014, Stockholm, Sweden) carried the significant contribution to the understanding of anomalous properties of liquid water. However, the problem of the clarification of the unusual properties of the water is still actual.

We present latest results of temperature evolution investigation of infrared absorption spectra of water in argon cryomatrix; to model phase transition from gas to condensed phase; to refer separate vibrational bands to different sized molecular clusters. After all, we can use these investigations results to explain temperature evolution of structure for condensed and solid phases of water under the normal pressure using the infrared spectra of condensed water recorded at different temperatures.

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Anomalous variation of phosphorescence of 2-BrBP with temperature: DFT computations and emission scenario

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The distinctive peculiarity of the phosphorescence spectra of crystalline ortho-bromobenzophenone (2-BrBP) is their variation with temperature [1]. The structure and other properties of 2-BrBP also have unusual peculiarities, among which are its propensity to form glass [2], existence of excimer [3], existence of a metastable phase [4] with the structure still unknown, etc. The main incentive of this research was to understand on the microscopic level the reason behind those unusual properties. To fulfil this task, the energy surfaces for states S_0, S_1 and T_1 were calculated as well as measurements were carried out using time-resolved phosphorescence (both in micro-second and nano-second regimes) and high-energy absorption techniques.

As results of DFT computations show, both excited states S_1 and T_1 have two physically meaningful minima. Since upon excitation to S_1 state the molecule very fast goes via inter-system conversion to the higher minimum of the state T_1, it is the latter that determines the scenario of the emission process. At low temperatures the molecule has insufficient energy to overcome the barrier to the deeper minimum, and thus emits at much shorter wavelengths. As the temperature is raised to 70 K or higher, the molecule finds its way over the barrier to the lower minimum and emit a monomeric series shifted significantly to red. At temperatures above 120-150 K the prevailing mechanism consists in the formation of a triplet excimer with the characteristic life times of a few tenths of a second.

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Stimulated raman adiabatic passage (STIRAP) in physics, chemistry and technology: Current status and future directions

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The original STIRAP paper was published in May, 1990 (J.Chem.Phys. **92**, 5363, 1990). Now, 25 years later, that methodology enjoys widespread application throughout a broad range of disciplines, including atomic, molecular and optics physics, nuclear physics, solid state physics, quantum information, chemistry and even technology. The talk will review the current status of STIRAP research and discuss anticipated future directions of STIRAP-related work. In particular, a special attention will be paid to the consequences of laser fluctuations on STIRAP efficiency.

International year of light and light-based technologies -2015: reflection in the mirror of Institute Physics NAS Ukraine

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The programs of International year of light 2015 promote improved public and political understanding of the central role of light in the modern world while also celebrating noteworthy anniversaries in 2015— from the first studies of optics 1,000 years ago to discoveries in optical communications that power the Internet today. This International Year should bring together many different stakeholders including scientific societies and unions, educational institutions, technology platforms, non-profit organizations and private sector partners.

The Opening Ceremony at UNESCO headquarter in Paris over 19-20 January 2015 launched the year-long series of activities all over the world. The XXII Galyna Puchkovska International School-Seminar “Spectroscopy of Molecules and Crystals” as well known spectroscopy meeting with many-years traditions is the important event of optical community in Ukraine in the frame of IYL2015.

We present here some milestones of Institute of Physics NAS Ukraine in optics and laser science since middle of twentieth century up to now. The optical spectroscopy as instrument of molecular crystals study was introduced into institute practices by academician Antonina Prikhotko at 40th and she has initiating the institute activity in the field of laser science and technology, nonlinear optics and holography. The examples of important results of more than half- century activity will be given in this presentation.

Scanning tunneling microscopy of organic monolayers on atomically flat surfaces

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Highly ordered organic films deposited on the solid surface are the subject of intense experimental and theoretical researches. In this talk the results of systematic STM-investigations of self-assembled monolayers of different organic compounds (n-alkanes, organic acids, n-alkanethiols, liquid crystals, fullerenes and organosilanes) on atomically flat surfaces will be presented. The results were obtained using scanning tunneling microscope (“NT MDT” and “Molecular Imaging”) adapted to the liquid environment. The highly oriented pyrolytic graphite and reconstructed Au(111) surfaces were used as the substrates. The observed structures are discussed in terms of molecule-molecule and molecule-substrate interactions.

Vibrational Spectroscopy as Probe of Structure and Dynamics of Heme Proteins

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Heme proteins are intensively used to study relationship between structure, dynamics and function of biological molecules.

It was shown in a number of our studies that the infrared absorption band, which corresponds to valent vibration of coordinated carbon monoxide of carbohmonoxy complexes of heme proteins, is extremely sensitive to electric field created by the heme environment.

Therefore, position and shape of this band and their temperture dependence can be succesfully used to reveal peculiarities of the protein structure and motin. In particular, it was shown that charachteristic times of motion of the heme environment is slower, than 0.1 ns.

2

Biomolecules & Polymers

Fluorescence dyes as guest molecules in model lipid membranes: DSC and UV-VIS spectrophotometry study

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Organic dyes are commonly used as fluorescent probes in biophysical and medical studies of membrane structure, dynamics and physiology. However, perturbations of the membrane properties by such probes may take place and thus probe-based experiments cannot be *a priori* considered as non-invasive. So, it is essential to have a deeper insight into eventual interference of the probe and lipid membrane [1].

In the present work three fluorescent dyes Rhodamine 6G, Rhodamine B and Acridine orange have been studied as guest molecules in model lipid membranes by differential scanning calorimetry and UV-VIS spectrophotometry techniques. The effect of the dyes on thermal behaviour of dipalmitoylphosphatidylcholine (DPPC) membranes (at 1:200 dye to lipid molar ratio) were found to be insignificant, as it is with the majority of guest molecules.

For Rhodamine 6G and Acridine orange, temperature-induced reversible changes of the absorption spectra were observed in lipid membrane media (as distinct from water solutions of these dyes). In the case of Acridine orange, the absorption spectrum transformation is in agreement with the changes in lipid membrane phase states. The effects are discussed in terms of dyes disaggregation with temperature due to increasing water and membrane solubility.

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Spectroscopic studies of DNA and RNA viruses

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Mosquito iridescent virus *Aedes flavescens* (AfIV) is a large (180 nm in diameter) 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 (60 nm in diameter) 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 the AfIV and IPNV virions as well as their nucleic acids and major capsid proteins in order to reveal the correlation between the composition of the two types of virions (different types of nucleic acids, different capsid proteins, presence and absence of lipid shells) and their spectral properties. Such a correlation might be a tool for distinguishing viruses of different type by means of optical spectroscopy.

Measured are absorption (UV), fluorescence, fluorescence excitation, phosphorescence and phosphorescence excitation spectra of the AfIV and IPNV virions as well as their nucleic acids and major capsid proteins.

The UV absorption of AfIV is shown to be due to absorption of all viral components (capsid proteins, lipids and DNA). AfIV virion fluorescence at room temperature is caused by the fluorescence of capsid proteins, while at low temperatures it is related to the fluorescence of both capsid proteins and viral DNA. The amino acid composition of the major capsid protein of the iridovirus is determined by means of sequencing the DNA fragment.

It is found that spectral properties of nucleic acids and major capsid proteins of the two viruses are considerably different while those of the whole AfIV and IPNV virions are similar.

Electron attachment to DNA-related biomolecules: studies combining photoelectron spectroscopy experiment and computational modeling

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It is well established that lethal effect of ionizing radiation in biological system results mainly from the appearance of the highly reactive hydroxyl and hydrogen radicals. In addition to above products of water radiolysis, secondary low-energy electrons (< 20 eV) are produced in large amounts.[1] Since discovery published in 2000, that dry plasmid DNA is highly susceptible to degradation by such low-energy electrons, the extensive studies have been devoted to the interactions between electrons and DNA.[2] In order to learn the details of DNA's response to electrons, we focused our efforts on determining of the intrinsic electrophilic properties of DNA components as observed in the gas phase.

Here, we present the results of combination of the photoelectron spectroscopy (PES) with quantum chemical calculations at the B3LYP/6-31++G** or M06-2X/6-31++G** level of theory applied to the anions of isolated nucleobases, nucleosides as well as their homodimers. PES provides a unique tool for observation of the stable, gaseous anion radicals and to determine their adiabatic electron affinities (AEA) as well as vertical detachment energies (VDE). In turn, computations allow to interpret the measured PES features. Theoretical approach involves considering all accessible geometries of investigated biomolecules and is based on the assumption that the most stable thermodynamically anion radicals are the structures which contribute to the PES. In fact, calculated VDEs and AEAs characterizing the most stable structures correspond well with the positions of the peaks in the PES.

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The peculiarities of the spectral properties of the biological systems.

Fundamental and applied aspects

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The spectroscopy of the biological systems is very interesting and important branch of physics. Namely the spectroscopy has a possibility to observe the response of the individual molecules and atomic groups in the biological systems.

In the present work

1) The spectral properties of synthetic organic molecules and biological molecules are examined. It is shown that in general, the spectral properties of these objects are the same and determined mainly by π-electron systems in the range from 1 to 1,6 eV. On the other hand, in a number of cases some specific spectral manifestation of the functional properties of the biological system is observed. Some examples of the specific electronic processes in polynucleotides and corresponding luminescent properties are examined and discussed.

2) It was examined what information can be obtained as the result of the investigation of the biological object spectral properties:

a) the individual spectral characteristics, the systems of energy sites, the possible quantum transfers, and electronic processes. Some examples concerning DNA, RNA and proteins are presented.

b) the spectral manifestation of the biological objects interaction and the proof of the small molecules binding to biological macromolecules.

3) The functional properties of biological macromolecules (manifested by luminescence spectra) invented by Nature are presented.

Exciton self-trapping in molecular aggregates formed in layered polymer films

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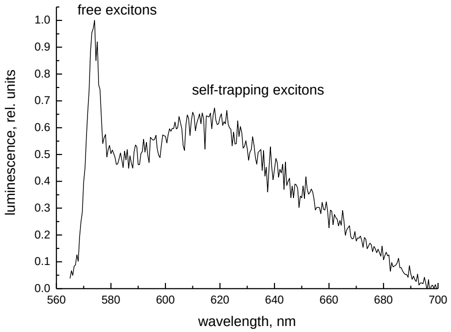
In recent decades, one of the most interesting objects for study of exciton dynamics in nanosystems are molecular aggregates of organic dyes, so-called J-aggregates. Due to unique optical properties such as small width of the spectral bands, extremely high extinction coefficients, record levels cubic susceptibility, etc. provided by delocalization of electronic excitations, J-aggregates are of great practical importance. Structure and optical properties of the J-aggregates are largely determined by their microenvironment, which can be used in the formation of J-aggregates with desired optical properties. One of the insufficiently studied phenomena in photophysics of J-aggregates is a self-trapping of excitons due to the strong exciton-phonon interaction. One of the main evidence of the possibility of excitons self- trapping in the J-aggregates is the appearance of their luminescence bands in the J-aggregate luminescence spectra at low temperatures. Analysis of the magnitude of the exciton-phonon interaction in J-aggregates of cyanine dyes series showed the possibility of the exciton self-trapping in some of them, even though it had not appear in the luminescence spectra at room temperature. In this paper, we report the observation of luminescence band of self-trapped excitons in J-aggregates of pseudoisocyanine (PIC) dye. PIC J-aggregates possess the weak exciton-phonon interaction in aqueous solutions and the exciton self-trapping in such case is impossible. It has been found that in a case of PIC J-aggregates formation in polymer films by method Layer-by-Layer assembly their spectral properties vary greatly as compared with the case of PIC J-aggregates formation in aqueous solutions. It is caused by changes in the structure of the J-aggregates: in place of the one-dimensional structure in solution, it becomes a quasi-three-dimensional in the film. As a result when cooled to liquid-nitrogen temperature the luminescence spectra reveals an emission of the self-trapped excitons. It is the first report of exciton self-trapping in PIC J-aggregates.



Multi-component structure of induction curve of chlorophyll fluorescence in wheat leaves

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The shape of induction curve of chlorophyll fluorescence in leaves of plants is caused by the several processes. They are the following: energy exchange in the light-harvesting antenna, photochemical transformation and an electron outflow from reaction centers. The shape of the induction curve becomes simpler when electron transport from the reaction centers is blocked because only energy exchange in antenna gives contribution.

In the present work an analysis of the shape of this curve is executed for leaves of 4 varieties of wheat. The original method is applied for analyzing the component structure of the induction curves by decomposing them into the exponents. The method uses the additional basis which is orthogonal in relation to the initial one. Step-by-step procedure is used for selecting the number of exponents, their amplitudes and decrements to obtain the best approximation of the experimental curve by the sum of these exponents. The procedure begins with approximation by a single exponent. Then the second one is added and their parameters are varied to reach the best optimization. An addition of components and the mutual adjusting of their parameters are repeated till obtaining the best approximation of the experimental curve. Thus, the novel information has been obtained in contrast to earlier researches who gave only amplitude values.

Revealing only three components in the analyzed induction curves is in a good accordance with finding out only three types of pigment-protein complexes in thylakoid membranes of chloroplasts. Thus, an analysis of induction curve of chlorophyll fluorescence can be used as an effective instrument for investigation of the state of photosynthetic membranes.

Spectral properties of the DNA in aqueous solutions saturated by hydrogen

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The optical spectroscopy methods (optical absorption, fluorescence and phosphorescence) are widely used in different biophysical investigations, especially for electronic structure investigations of biomacromolecules such as the deoxyribonucleic acid (DNA). The DNA electronic properties are connected with presence of pi-electronic groups in DNA strands and manifested in the optical wavelength range (near "biologic" ultraviolet, visual and near infrared). This fact gives the ground to apply optics spectroscopy for the DNA electronic structure study. Fluorescence and phosphorescence quantum yield of the majority of biological pi-electron-containing compounds is small at normal conditions therefore their fluorescence and phosphorescence are investigated substantially at low temperatures. Additionally, triplet excitations are captured by oxygen from solution at normal conditions that causes phosphorescence quenching. As the result, phosphorescence can normally be observed in rigid matrices (at low temperatures) or degassed solutions.

The present study shows the results of spectral investigations of the DNA in aqueous solution saturated by hydrogen. We believe the hydrogen have reacted with the oxygen from solution thus this solution can be considered carefully degassed. The phosphorescence of the DNA in the degassed solutions at room temperature was observed (contrary to the solutions not degased) under excitation by wavelengths 240-300 nm, the phosphorescence spectra curves practically coincide for all excitation wavelengths from the range. These data resemble with our previous data on phosphorescence investigations at low pressure: the phosphorescence of the DNA powder at the air pressure P= 10 mm Hg over the DNA sample was observed at room temperature. The comparative studies of the DNA in aqueous solutions saturated by hydrogen and the DNA in aqueous solutions (not degased) show that phosphorescence spectra of both these types of solutions at T=77K practically coincide. The influence of hydrogen on the DNA aqueous solutions and separately on the DNA strands is discussed.

Intermolecular interactions in solutions of some analgesic drugs

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2,2’,2’’,2’’’-[(4,8- di(piperidin-1-yl)-pyrimido-[5,4-d]-pyrimidine-2,6-diyl) bis (azanitriyl)-tetra ethanol and (RS)-2-(4-methy,propyl propanoic acid some derivatives of salicylic acid and ibuprofen, were analyzed from the point of view of their interaction with solvents.

A solvatochromic study emphasized the presence both of universal and specific interactions in solutions of the analgesic compounds.

The electro-optical parameters of the studied molecules were established by quantum mechanical calculations.

The results obtained by quantum mechanical studies and also by solvatochromic evaluation, were used to compute the molecular parameters in the excited state of the spectrally active molecules.

This kind of studies is important for Quantum Chemistry due to their contribution to the Data Base regarding the microscopic parameters in the excited states of the molecules.

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Spectral and photophysical properties of rhodamine and pyrromethene dyes in new aliphatic polyurethane matrix

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To develop the dye-based laser elements, various solid-state matrices, such as polymers, porous glasses, polymer-doped porous glasses, and sol-gel materials, are used. Pure polymers are distinguished by their diversity, availability, cheapness, ability for easy dye doping, and homogeneity. The matrices should provide sufficient beam strength, transparency, high solubility of dyes, and dye stability during storage and operation.

The aim of the present work is investigations of the probability for the aliphatic polyurethane (APU) to be used as a efficient polymer matrix in the development of dye-doped active laser media. This work deals with the laser perspective dyes, namely, widely used Rhodamine 6G (Rh6G), and also pyrromethene dyes, PM567 and PM597. Spectral properties of these dyes in this matrix have been shown to be the same as in the liquid media (methanol, ethanol).

The photodecay of Rh6G, PM567 and PM597 dyes in the APU and polyurethane acrylate (for a comparison) matrices have been investigated by irradiation experiments by means of a DRK-120 lamp and second harmonic continuous generation of a neodymium laser (532 nm).

Laser active elements based on APU significantly exceed the ones made of other polymer matrices by photostability. The main reason for the high photostability and operation lifetime of laser APU-based active elements was shown to be the absence of reactive radicals. The results of this work allow to make a conclusion about good prospects for the applications of the active laser media based on aliphatic polyurethane in the development of tunable dye lasers.

Structure effects of diisocyanate on molecular dipole moments of isolated molecules and their dimer associates

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The important factor, affecting photooptical properties of solid-state dye laser elements based on elastic polyurethane matrices is their dielectric permeability. This value depends on the polarity of both glycol and diisocyanate components. Significant influence on the properties of segmented polyurethanes is caused by the processes of microphase exfoliation due to the association of fragments, bounded with the isocyanate part.

Polarity of the diisocyanate component in the polyurethanes based on oligo-diethylene glycol and diisocyanates of different structures has been studied by means of computer simulation of molecular structure by the PM3 semiempirical method with geometry optimization. Molecular dipole moments of different structure diisocyanates, 2,4- and 2,6-toluene diisocyanate (TDI) and hexamethylene diisocyanate (HMDI), have been calculated and analyzed, taking into account the effects of fragment association for both cases of isolated molecules and their dimer associates.

The results have shown that conformational flexibility of the HMDI methylene chain is the most favourable factor for the associate formation with high values of molecular dipole moments.

Investigated spectral and photophysical properties of phenalenone dyes in the polyurethane matrices correlate with polarity values of the diisocyanate component, which high dipole molecular moment causes high polarity of the polymer matrix, in its turn, providing an increase of Stokes shift and dye photostability due to efficient solvation processes.

Optical activity of polymer solutions studied by visible electron spectroscopy

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Current trends in Physics-Chemistry are focused on investigation of hydro-soluble polymers for biomedical purposes. In this context, optical and spectral properties of the macromolecular compounds are essential for designing materials that interact in a specific manner with electromagnetic fields as a result of the structural peculiarities. Some polymer solutions can turn the polarization plane around the light propagation direction.

The rotation angle θ is expressed as $\theta = [\theta] \cdot C \cdot L$, where $[\theta]$ is the specific rotation, C is polymer concentration and L is the thickness of the solution layer. The specific rotation is directly proportional with the circular birefringence ($\Delta n_c = n_l - n_r$) of the polymer solutions. The rotation angle of the polarization plane caused by a unitary layer is defined by $[\theta] = \pi \bar{\nu} \Delta n_c$. The irrespective refractive indices are measured with circularly polarized radiations to left, respectively to right.

The purpose of our research was to determine the circular birefringence of some poly (propylene oxide) (PPO) and hydroxyl propylene cellulose (HPC) in different solvents, in order to explain the role of solvent in the optical rotatory process.

The obtained results are useful in interpretation of the factors related to the conformational changes induced by the solvents’ nature.

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Calculation of thermodynamic parameters of ligand to DNA binding from the temperature dependences of visible spectra

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Knowledge of thermodynamic profile of ligand complexation with nucleic acids is important for understanding the mechanism of medico-biological action of the currently existing drugs and for designing of new drugs with improved medical effect. We propose the novel method to calculate the binding parameters in the DNA-ligand system. It is based on the equations of chemical equilibrium for analysis of spectrophotometric data in the wide range of temperatures (20-90^{0}C). In this temperature range it is necessary take into account the melting of DNA-ligand complex. The melting of complex we consider as two independent equilibrium processes: the complex dissociation and the DNA denaturation. The high-polymer DNA macromolecule represents as an assembly of cooperative units that melt by two-state model. The complex dissociation is described as stepwise saturation of the cooperative unit by the ligand molecules. In the approach the temperature dependences on the melting and binding enthalpies as well as the constants of these processes are taken into account.

Such approach enables to extract the binding constant, stoichiometry, enthalpy, entropy, and heat capacity changes from temperature dependencies on DNA-ligand complex absorption in the visible spectral region.

Using this method, we calculate the binding parameters of berberine (Be), methylene blue (Mb) and proflavin (Pf) with salmon testes DNA. The follow values are obtained: $K_{Be} = 1*10^5$ M^{-1}, $\Delta H_{Be} = -10$ kcal/M; $K_{Mb} = 7*10^4$ M^{-1}, $\Delta H_{Mb} = -4$ kcal/M; $K_{Pf} = 1{,}5*10^5$ M^{-1}, $\Delta H_{Pf} = -5{,}2$ kcal/M. These values are corresponding to the binding parameters for intercalation mode.

The MDA-MB-231 cells affected by different types of nanoparticles studied by confocal Raman microspectroscopy

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The cells of human breast adenocarcinoma (MDA-MB-231 cell-line) were studied by means of confocal Raman microspectroscopy. Samples contain cells affected with carbon nanotubes, gold and ferum nanoparticles and control cells which were not affected. The cells were deposited on thin glass slides and fixed by fixed agent in order to eleminate their mobility and influence of the external environment. Measurements were carried out using the spectrometer T64000 (Horiba, Jobin Yvon) in backscattering geometry. The excitation source was Ar-Kr laser (Spectraphysics) with wavelength 514,4 nm. The confocal microscope BX41 (Olympus) was used to focus the laser beam on the cell and to obtain responding signal from the sample.

It was found that fluorescence background from the fixing agent is very intensive. Therefore, we irradiate each cell for 2-3 minutes before the start of the acquisition. The obtained spectra indicate, that the light with the wavelength 514,5 nm completely absorbed by the cell membrane (similar situation is observed for a laser wavelength 488 nm). The spectra of all specimens have significant similarity to the spectra of the phosphatidylethanolamine [1] and phosphatidylcholine [2].

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I-type collagen fluorescence spectroscopy

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Living tissues are composed of cells embedded in extracellular matrix, the latter mainly consisting of proteoglycans, collagen and elastin. Collagen is the main load-bearing component within the tissue, while the elastin provides elasticity to the tissue and the proteoglycans give the tissue its swelling capacity. In load-bearing tissues collagen is abundantly present and the mechanical properties depend on the collagen fibre architecture, e.g. collagen fibre orientation, collagen fibre content and collagen fibre crosslinking.

The diagnostics of living tissues without the use of specific probes through different techniques have been the subject of an extensive study. Main goal for fluorescence diagnostics is to identify fluorescence features that can be used to identify/classify tissue as normal or diseased. Studying the active change in I-type collagen fluorescence with the changes of its state and architecture is the focus of the present work.

We studied the emission of I-type collagen fluorescence in bovine tendons in its native wet state and dried one. Samples were prepared in sections perpendicular and parallel to fibres, also the powder of dried tendon with the destroyed fibre architecture was prepared for the comparison. The emission spectra were recorded in different areas of the same sample. In fluorescence spectra of all the samples three kinds of emitting species were manifested with the maxima of fluorescence and emission spectra 280 and 320 (corresponding the most possibly to tryptophan and tyrosine emission), 350 and 420, 460 and 500 nm respectively. This fluorescence is provided mainly by collagen content. It is noticeable that the state of collagen affects the shape and intensity of the fluorescence spectrum. Measurements on tendon collagen show that the structure of the system, strongly influenced by protein-water interaction, determines the spectral properties of collagen fluorescence.

Relaxation spectra of aqueous solution of human serum albumin

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Temporal characteristics of structural and thermal relaxation have been determined in the present paper for aqueous solution of human serum albumin (HSA) using the measurements of sound attenuation spectra and the simulations of molecular dynamics with pressure and temperature jumps. The intercorrelated spectral analysis based on a maximum entropy method has been applied to all the relaxation curves and seven discrete processes of molecular relaxation with characteristic time constants differing by six orders of magnitude (from 0.5 ps to 0.5 µs) have been defined.

We have shown that the fastest two among the relaxation processes were caused by breaking of the hydrogen bond (0.5 ps) and reorientation (1.5 ps) of the undisturbed water molecules in bulk solvent. Two slower processes corresponded with two phases of dynamics of water molecules in the protein hydration layer. One of them (5-10 ps) have been attributed to the changes of orientation of the water molecules in the close vicinity of the protein surface and the other one (40-100 ps) have been done to the transitions of water molecules from hydration layer to bulk solvent, these transitions do not change the total number of hydrogen bonds of water in the system. The next two relaxation processes define dynamics of two phases (0.5-2 ns and 3-20 ns) of the global cooperative unfolding of the protein globule that is accompanied with hydration changes and is temperature dependent. The slowest (80-150 ns) among determined relaxation processes has been assigned to conformational transition, which occurs without globule unfolding and is caused by local mobility of α-helixes located in the inaccessible for water protein interior; this conformational transition has been found temperature independent and entropy driven.

Relaxation spectra human serum albumin complexed with ligand

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In the present paper the effect of binding of two low molecular ligands, which differ by their functional nature, on equilibrium state parameters and relaxation dynamics of human serum albumin (HSA) in aqueous environment has been studied. One of the ligands was represented by endogenous compound - myristic acid and another one was anticoagulant drug warfarin. Temporal occurrences of structural relaxation after pressure jump in the ligand-protein-water systems have been established on the basis of molecular dynamics simulation. Changes of the relaxation behavior of the protein have been found as a result of ligand binding. These changes have been characterized in terms of molecular structure and internal dynamics of protein globule and their correlation with thermodynamic parameters of ligand - protein binding have been defined.

We have shown that discrete components related to the processes of local and global conformational changes of protein as well as various phases of mobility of bulk and hydration water molecules can be identified in the relaxation spectra of the studied systems. In particular, it has been ascertained that binding of both endogenous and exogenous ligands with HSA results in drop of all frequencies of conformational transitions determined in the study and in reduction of residence time of water molecules in the protein hydration layer. Besides, we have shown predominance of entropy effect in binding thermodynamics of heterogeneous ligands with human serum albumin that should be taken in consideration when selecting factors of regulatory influence on the protein, for instance, under drug design. The found regularities of conformational dynamics of HSA and ligand-HSA complexes can be used in development of methods of medicinal chemistry and prediction of pharmacokinetics of drugs. In addition, the obtained data form the basis for decoding molecular spectra of protein solutions obtained by various experimental methods in time interval from 0.5 ps to 0.5 μs.

Spectroscopic studies of plastics welded joints

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As it is known polyethylene (PE) and polypropylene (PP) are the mostly common polymer materials in the modern world, and their products take the major share on industrial and trade markets. For example, various types of technical PE like PE-63, PE-80 and PE-100 as well as PP have wide industrial applications, i.e. in construction, for pipeline systems etc. A rapid development of plastics industry limits detailed investigation of welding processes and welds' formation mechanism; so they stay unrevealed. There is still no final answer to the question how weld's microstructure forms. Such approach limits our way to the understanding of the problem and, respectively, prevents scientific approaches to the welding of more complicated (from chemical point of view) types of polymers than PE and PP, such as polyetherimide (PEI) and polyetheretherketone (PEEK).

In this work the complex structural and thermophysical properties of PE, PP, PEI, PEEK and their welded joints obtained by various welding techniques, such as butt welding with heated tool, thermoresistive and ultrasonic welding are studied by wide-angle (WAXS) and small-angle (SAXS) X-ray spectroscopy, differential scanning calorimetry (DSC) and thermomechanical analysis (TMA).

As one of the results it is revealed that during the welding process of PE restructuring of crystalline phases occurs, and crystalline areas with higher mechanical and thermal properties appears, due to increase of quantity of crystallites, and to their bigger size and better ordering (packing).

Spectroscopic studies of solid polymer electrolytes based on epoxy oligomers and lithium perchlorate salt

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In the present work ion-conductive hybrid organic-inorganic polymers based on epoxy oligomer of diglycide aliphatic ester of polyethylene glycol (DEG) and lithium perchlorate ($LiClO_4$) were synthesized. The effect of $LiClO_4$ content on electrophysical properties of epoxy polymers has been studied by Differential Scanning Calorimetry (DSC) and Broadband Dielectric Spectroscopy (BDS). The effect of $LiClO_4$ content on structure has been studied by Wide-Angle X-ray Scattering (WAXS). It was found that lithium perchlorate impacts on structure of the synthesized hybrid epoxy polymers, probably, by formation of coordinative complexes {ether oxygen - lithium cations - ether oxygen} as evidenced from a significant increase in their glass transition temperatures with increasing $LiClO_4$ concentration and WAXS studies. The presence of ether oxygen in DEG macromolecules provides a transfer mechanism of the lithium cations with the ether oxygen similar to polyethylene oxide (PEO). Thus, the obtained hybrid polymers has high values of ionic conductivity σ' (~10^{-3} S/cm) and permittivity ε' ($6\cdot10^5$) at elevated temperatures (200 ^{o}C). On the other hand, DEG has higher heat resistance comparing to PEO that makes these systems perspective as solid polymer electrolytes able to operate at high temperature.

Luminescence under X – ray excitation of keratin samples as a function of temperatures

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The luminescence of the keratin (human hair and nail plates) was investigated as a function of temperature between 8 K and 350 K under X – ray excitation. Female hair and whole nail plate without mechanical and chemical damage were used in experiments. Hair was fitted in the measuring cell and compressed to decrease layer of air between them, cross section of cell was irradiated. For experiments with nail plates irradiation was carried out on the inner side of plates. Each experimental sample for luminescence under X – ray excitation (XRL) researches was irradiated by X – ray tube БХВ – Re (20 kV, 25 mA). Light from sample was detected in visible region by the FEU – 106 photomultiplier. Spectral measurements were carried out using a monochromator MDR – 2.

The spectra of XRL of hair and nails have a non-elementary form in spectral region from 350 to 550 nm. The observed spectra of XLR for nails have one broad band with the maximum of luminescence at 450 nm for all range of experimental temperatures. As for XRL spectra of hair for 293 K the maximum of luminescence was observed at 550 nm and for 85 K was registered second maximum at 450 nm.

In temperatures range from 300 K to 8 K the luminescence intensity of keratin samples increases.

It is pertinent to note that the intensity of XRL for experimental samples is weak compared to classical luminophores (for example ZnS-Cu). That is due to factors: a low absorption coefficient of X – radiation and optical heterogeneity of keratin samples that leads to scattering of luminescence radiation.

EEET and Peculiarities of Light-Emitting Layers Design for White OLED

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From the first well-known publication about the organic light-emitting devices (OLED) in 1987 [1] researchers made a huge progress in this field. In fact, the progress is so strong that nowadays we have a lot of devices using OLED-screens like cell-phones, OLED-TVs or light-panels [2]. However, the family of OLED technologies still has some problems which needed to be solved to allow OLEDs to compete with classical lighting and display technologies. Efficiency is one of them.

In our research we focus on the investigations of polymer/dye emissive layers characteristics and peculiarities. Such emissive layers have some notable potential advances like flexibility, transparency, the ability to create white light with just one emissive layer etc. In such systems typically there is an electronic excitation energy transfer (EEET) from polymer matrix to emissive dyes. The efficiency of this EET is a subject of great importance because it’s directly influence the common efficiency of the device.

To evaluate the characteristics of EET in such systems we used two different approaches: Powell’s model, developed by Slobodyanik and Yashchuk [3, 4] and Faidysh diffusion model [5]. Both models allow one to estimate the number of exciton jumps in the matrix before its deactivation using luminescence intensity data. The number of jumps thus can be used to estimate the length of exciton travel before its deactivation which leads us to the average value of optimal concentration of the dopant.

As a result of this work the values of effective concentrations of the emissive dopants were estimated for a number of polymer/dye films with polyepoxypropilcarbazole (PEPCa) and polystyrene (pS) as oligomer and polymer matrices respectively. This method allows us to evaluate the most effective dopant concentrations in the polymer/dye systems in the context of excitation energy transfer and thus to improve efficiency of such systems.

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The spectral properties of the telomere fragments

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The telomere is the end part of the deoxyribonucleic acid (DNA) – the biomacromolecule that is vitally important for any living creature. The telomere contains the large number of repeated sequences of 6 nucleotides TTAGGG (for vertebrates). The main role of telomeres is the DNA protection. Absence of telomere leads to the loss of important genetic information and the shortening of chromosomes that can lead to apoptosis. The telomeric DNA is shortened during cell growth of the human body. However, for cancer cells such shortening does not occur, because of the high (compared to normal cells) activity of the telomerase enzyme that synthesizes the lost telomeric sequences. Thus, the main task of modern anticancer strategy is the methods invention of control and violation of processes in which telomere takes part. The telomere contains pi-electron groups as well as DNA, thus it gives the ground to apply optics spectroscopy for the telomere electronic structure study.

The optical absorption, fluorescence and phosphorescence (including low temperatures measurements) of telomere fragment – oligonucleotide d(AGGGTTAGGGTTAGGGTTAGGG) and the DNA macromolecule were investigated under various excitation wavelengths (240-300 nm). It was shown the absorbing centers in d(AGGGTTAGGGTTAGGGTTAGGG) as well as the DNA macromolecules are the basic groups. To the other hand, the phosphorescence spectra of this oligonucleotide are close to the correspondent DNA spectra and practically do not depend on excitation wavelength from the range. It gives the ground to conclude that main triplet electronic excitations traps in d(AGGGTTAGGGTTAGGGTTAGGG) as well as the DNA are the complex formed by adenine (A) and thymine (T) chromophores. The phosphorescence/ fluorescence maxima intensities ratio of d(AGGGTTAGGGTTAGGGTTAGGG) increases dramatically comparing with such ratio of the DNA. The ratio increasing reasons are discussed. The fact of the ratio increasing can be basis for the method of the telomere detection inside the DNA.

Hydration of model membrane surface in the presence of drugs by the evidence of FTIR-spectroscopy

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Extreme importance of hydration for all biological processes [1] gives rise to permanent interest in studies of water structure in various biological objects, viz., in lipid membranes. Model *L*-α-dipalmitoylphosphatidylcholine (DPPC) membranes with drugs admixtures (“Noobut IC”, “Amixin IC”, “Erespal” etc.) were examined by FTIR spectroscopy (“Spectrum One”, PerkinElmer). For the broad water band νO–H 3400 cm^{-1}, a Gauss deconvolution into three peaks were performed according to [2]: ~3100 cm^{-1} (ν_1O–H), ~3500 cm^{-1} (ν_3O–H) and ~3600 cm^{-1} (disturbed, or “multimer”, water). Both position and fraction of symmetric ν_1O–H and antisymmetric ν_3O–H bands were shown to be affected by the presence of drugs, whereas the corresponding values of “multimer” water remained almost unchanged. Interesting is that drugs admixing to DPPC membranes results in elevation of ν_1 fraction and simultaneous decreasing of ν_3 one. Meanwhile, in water solutions of the same drugs the picture was inverse, with ν_3 vibrations being preferable. One can conclude that drugs are able to modify hydration parameters of the membrane surface, though the contribution of the membrane surface itself remains determinative.

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The DNA phosphorescence: the conditions of AT-complex formation

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The deoxyribonucleic acid (DNA) is the well known biological macromolecule that is vitally important for all living organisms. It plays main role in storage of genetic information and is the smallest building block of any living cells. DNA fragments are parts of antiviral and antitumor drugs. The processes of the development of any living creature are closely connected with the DNA electronic structure and its changes. Thus, the study of electronic properties of the DNA and interaction between its structural units are an important task of the modern science. Such properties are connected with presence of pi-electron groups (chromophores) in the DNA strands and manifested in the optical wavelength range (near "biologic" ultraviolet, visual and near infrared). This fact gives the ground to apply optics spectroscopy for the DNA electronic structure study.

Our previous studies showed that main triplet electronic excitations trap (responsible for phosphorescence) in the DNA is the complex formed by adenine (A) and thymine (T) chromophores. The present study shows the spectral investigations results of specific conditions of this complex formation. The optical absorption, fluorescence and phosphorescence (including low temperatures measurements) of A and T monomers, their mixtures and the DNA macromolecule were investigated under various temperatures of the mixtures preparation (in the temperature range 323-353K) and excitation wavelengths (240-300 nm). There were studied two types of the solutions mixtures prepared: the first type of the mixtures after having been prepared was frozen immediately to low temperatures and investigated; the second type was slow getting cold together with thermostating surroundings and after some time investigated. The changes of the mixtures phosphorescence spectra bands were fixed depending on the conditions mentioned above. It was noted that effective AT-complex formation started at T=343K of the mixtures preparation. The mechanism of this complex formation is discussed.

Study of the interaction of iron (II) clathrochelates with globular proteins

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Iron (II) clathrochelates - cage complexes with encapsulated metal ion are intensively studied for their interaction with biomolecules. These compounds have shown their ability to bind with serum albumins that results in the protein fluorescence quenching and induction of the bands in the CD spectra in visible spectral region. The most pronounced response on the presence of the albumins was demonstrated by the compounds containing ribbed thiaphenyl carboxy substituents.

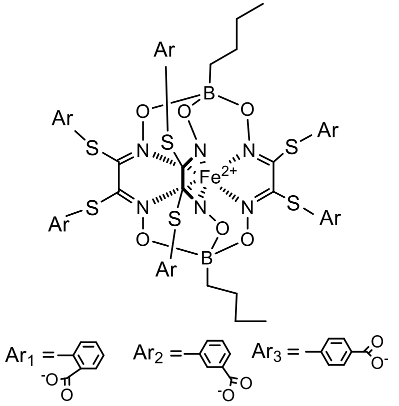

Fig.1. Structure of clathro-chelates ortho-(Ar_1), meta-(Ar_2), para-(Ar_3) positions.

Here we report study of the interaction between hexa-substituted thiaphenylcarboxy clathrohelates (orto-, meta-, para- isomers, Fig.1.) with globular proteins bovine (BSA), human (HSA) serum albumins, β-lactoglobulin (BLG) and insulin (INS) using protein fluorescence quenching and circular dichroism (CD) methods.

The presence of clathrochelates leads to the quenching of protein fluorescence from 2-3 times for BLG up to 12-15 times for BSA that evidences interaction between the cage complex and protein.

Under binding to proteins cage complexes induced CD bands in range 350-550 nm, while intrinsically these compounds don’t possess optical activity. The intensity and shape of CD spectra depend on the kind of both isomer and protein. The most intensive bands are observed for orto-, meta- and para isomer in the presence of BLG, BSA and insulin respectively. The appearance of the optical activity of clathrochelates in the presence of protein is explained by the fixation of metal coordinated polyhedron in its twisted conformation in the formed complex.

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Functional luminescent carbazole-containing compounds for power saving light sources

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One of the main problems of the natural resources conservation is the saving of electrical energy the main part of which is utilized by light sources. That is why the design of novel functional materials for high effective energy saving source of light is in the special interest of the modern technology world.

In our report the investigation results of the optical absorption and luminescence properties of vinylaromatic carbazole-containing compounds (designed for high effective electroluminescent devices production) are presented. The compounds investigated contain one, two, five and six carbazole pi-electron groups. The optical absorption and luminescence of these compounds in solutions, powders and films were studied at 293K and 77K. The effect of various deposition technologies of these compounds films on their luminescence spectra were fixed and discussed. It is proved the energy structures of these compounds are determined mainly by π-electron systems of carbazole groups and the weak interaction between them exists. The nature of luminescence of the investigated compounds is discussed. The investigated compounds films manifest the main impurity contribution in their fluorescence and phosphorescence spectra contrary to their correspondent solutions spectra. In a number of cases the influence of π-electron groups each other leads to domination of phosphorescence in luminescence spectra. The effects of difference in deposition technology on spectral properties of investigated compounds as well as their applications in OLEDs are discussed.

Research photovoltaic effect in the structure of squaraine dye and fullerene C_{60}

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Over the past decades scientists and engineers have done a great amount of researches in two directions: improve the efficiency of solar converters and their reduction in price. By using silicon solar batteries the problem is the high price – up to 300-420 euros per m^2 of surface, as pure monocrystalline silicon is difficult and expensive to produce [1].

Another option is to use photovoltaic elements are based on films of organic materials that, although have relatively low efficiency (~5%), would be cheaper compared to silicon technology [2].

Reason for the lack of efficiency of solar cells is relatively narrow absorption spectrum, low open circuit voltage and, in many cases, low filling factor – is the main problem of their future application in practice. Therefore, the study of the processes occurring in the elements of organic materials in order to improve efficiency is one of the urgent problems nowadays.

By the thermal vacuum deposition technics, the layer wise photovoltaic cells squarine dye/C_{60} were fabricated. The absorption spectrum of thin films of squarine dye, C_{60} and their layer wise structure were obtained as well.

Motorized system that allows you to move remotely the mask for spraying without disturbing the vacuum in the deposition process was developed and produced.

We derived photovoltaic parameters of our elements. For the best of them, an open-circuit voltage was 380 mV. The open-circuit voltage dependence of the wavelength was obtained.

By virtue of atomic-force microscopy we acquired the results which shows us that fullerene’s film surface is a quite uniform, despite of dye’s film that is susceptible to form island surface.

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Graphene enhanced infra-red absorption (GEIRA) effect from biological molecules

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Nowadays sensing of biological agents requires new materials as substrates for the detection low amount number of molecules. Special scientific hopes are placed on surface enhanced spectroscopy techniques using electromagnetic and chemical influence of surfaces for enhancing of Raman or infrared signals. Graphene and graphene oxide materials can be used as a new platform for Surface Enhanced Infrared Absorption Spectroscopy, because of their unique properties: unique electron and phonon structures, atomic uniformity and biological compatibility.

Graphene enhanced infrared absorption (GEIRA) effect was studied by us for graphene for the first time. This effect was carried out for adenine adsorbed on graphene layers.

Infrared spectra have been registered with IFS-66 Bruker instrument in the 400-5000 cm^{-1} region. The maximum enhancement factor for adenine on graphene layers equal to 5 and for thymine equal to 4 respectively.

Mechanism of enhancement of thymine and adenine molecules adsorbed on nanostructured carbon substrates seems to have chemical and electromagnetic nature. Electromagnetic mechanism could be connected with excitation of plasmon vibrations in graphene layers in THz and infrared region, while chemical mechanism depends on a strong interaction between molecules on graphene

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Spectroscopic studies on binding of porphyrin-phenazine conjugate to poly(G)

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Binding of a novel cationic porphyrin–imidazophenazine conjugate, TMPyP^{3+}–ImPzn, to four-stranded poly(G) was investigated in aqueous solutions of neutral pH under near physiological ionic conditions using absorption, polarized fluorescent spectroscopy and fluorescence titration techniques. In absence of the polymer the conjugate folds into stable internal heterodimer with stacking between the porphyrin and phenazine chromophores. Binding of TMPyP^{3+}–ImPzn to poly(G) is realized by two competing ways. At low polymer-to-dye ratio ($P/D < 6$) outside electrostatic binding of the cationic porphyrin moieties of the conjugate to anionic polynucleotide backbone with their self-stacking is predominant. It is accompanied by heterodimer dissociation and distancing of phenazine moieties from the polymer. This binding mode is characterized by strong quenching of the conjugate fluorescence. Increase of *P/D* results in the disintegration of the porphyrin stacks and redistribution of the bound conjugate molecules along the polymer chain. At $P/D > 10$ another binding mode becomes dominant, embedding of TMPyP^{3+}–ImPzn heterodimers into poly(G) groove as a whole is occurred.

Luminescent solar concentrators based on perylene dyes absorbed on nanoparticles of aerosil and zinc oxide dispersed in polymer matrix

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Solar energy is one of the most attractive areas of research related to the exploration and development of unconventional technical clean and cheap energy sources as an alternative to nuclear and thermal power. Low density of solar radiation at the earth's surface is a limitation to the wider use of its. In order to surmount this obstacle, it is necessary to employ solar energy concentrators. Concentrators based on parabolic and cylindrical mirrors have significant drawbacks, such as a system for tracking the position of the sun, high wind resistance, wind resistance requires powerful attachment, fast and very dusty mirrors reflecting surface. Moreover, such concentrators do not work in overcast weather conditions. Luminescent solar concentrators (LSCs) are free from all these disadvantages. Our most recent review of publications on this subject can be found in [1].

Our current presentation is devoted to the investigation of luminescent properties of several perylene dyes absorbed on inorganic nanoparticles dispersed in polymer media, which can be potentially used as a matrix for manufacturing LSCs. Nanoparticles of aerosil (size from 16 to 40 nm) and zinc oxide (mean size 15 nm) were treated with solutions of perylene dyes, such as Lumogen Red 300, Lumogen Orange 240 and Lumogen Yellow 83 in organic solvents following by their incorporation in poly(vinyl pyrrolidone), polymethylmethacrylate and copolymers of methyl acrylate and aliphatic cyanoacrylates. The quantitative assessment of the relative quantum yields of fluorescence for dye-containing inorganic nanoparticles in their aggregated form and their aggregate-free form after dispersion in polymer media is performed and possible explanation of enhanced fluorescence in case of polymer-based nanocomposites is discussed.

[1] V. M. Granchak, T. V. Sakhno, S. Ya. Kuchmy // Theoretical and Experimental Chemistry, 2014, V. 50, No. 1, C.

Conformational changes by double photoinduction in the purple bacteria reaction centers

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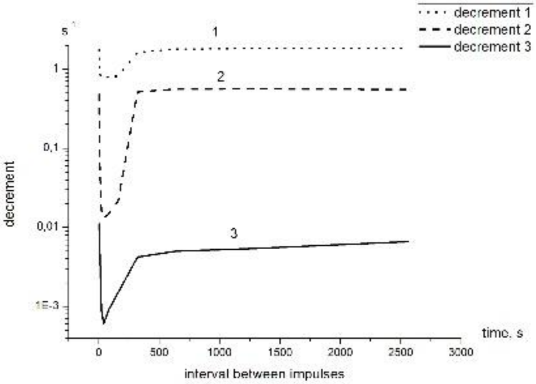
The reaction center (RC) structure is well studied. It has high efficiency of photogeneration. RC can be used as an element of nanoelectronics and as a part of the artificial photosystems.

In the process of photoinduction, there is charge transfer from the donor (bacteriochlorophyll) to the secondary acceptor (ubiquinone). It provides the existence of a long charge separation state, which creates transmembrane potential. The charge transfer in the RC is accompanied by structural changes as the result of electron-conformational interactions. Thus, electron transfer can be an indicator of structural changes in the RC. The electron transfer kinetics of the RC solutions studied by light absorbance measuring at 870 nm wavelength. As a result, dependencies of the absorption coefficient changes at various intensities and photoinduction durations were obtained. Return of the electron from the donor to the acceptor after turning off the light does not necessarily lead to RC structure recovery to the dark-adapted state. Therefore, we propose a method of RC dual photoinduction with different intervals between the impulses. The kinetics of the RC recovery after the second impulse was analyzed with exponential decomposition.



After 60 s photoinduction with light intensity of 6 mW/m^2 RC returns to the dark-adapted state in 500 s after turning off the light. There is a significant slowing down of the relaxation kinetics in the RC recovery process when intervals between light impulses are less than 40 s. After dual photoinduction without interval electron return is faster than after the double impulse with interval up to 40 seconds. It can be explained by the additional excitation of the local vibrational modes in a limited volume (fractons amplification) as the result of the second impulse.

Infrared spectrum of residues formed in the process of biofuel production before and after oxidation within the electrochemical generator

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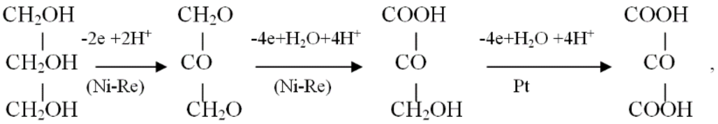
Biofuel production has increased throughout the world, which had been caused both by low price (it is 1,5 times cheaper that fuel) and its environmental friendliness; a microorganism processes 99% of fuel per month.

We have examined residues formed before and after biofuel generation not only as a source of power production, but as compounds, which in the process of electro-oxidation turn into substances possible for future use in different operations.

Previously residues were examined on a chromatographical basis. Electro-oxidation was performed in a usual glass cell with parted anode and cathode chamber in 7 m KON. Pt and Ni-Re were involved as an anode, and spinel NiCo2O4 was used as a cathode. The “skinning” method (glass KRS-5, spectrometer - Spekord) was applied for removal of infra-red spectrum. The residues under examination are characterized by a broad absorption band in the range of 2900-3500 cm^{-1} and less intensive absorption band 15600-1540 cm^{-1}, 1410-1380 cm^{-1}, which alongside with chromatographical researches allowed to define the residues under examination as glycerin (98%), containing esters of methyl and ethyl acid.



I II III

After having been oxidized infra-red spectrum is characterized by a sharp change of the absorption band in the range of 2900-3500 cm^{-1}, appearance of a narrow band 1700-1730 cm^{-1} and intensity of lines in the range of 800-1400 cm^{-1}. The research, we have conduct, allowed to establish the following scheme of transformation of residues over catalysts Ni-Re and Pt, as well as to determine that residues formed after biofuel generation can be used in a electrochemical generator (7M KOH; T=333-353; I=10 mA/ cm^2) and can serve for obtaining products applied in the industry (T oxy-2- propanol – a solvent medium for cellulose nitrate; an ingredient of tanning lotions, emulsifiers, an accelerant for ester synthesis; II – pyroracemic acid, used in biochemical researches; III – ketomalonic acid – an accelerant in organic synthesis).

Photovoltaic and photophysical properties of thin film polyvinyl alcohol based composites doped with chromium (III) organic complexes

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The new photoconductive film composites based on polyvinyl alcohol doped by high concentration of chromium (III) complexes have been prepared. Their electric, photophysical and photovoltaic properties are investigated. The photoelectric properties of obtained composite films have been investigated by Kelvin probe method of surface electric potential measurement. It was shown, that investigated film composites exhibit photovoltaic properties under illumination by light from the complexes absorption region. The kinetic behavior and spectral dependence of the observed photovoltaic effect was studied. The nature, mechanism and features of the photovoltaic effect in the investigated film compositions are discussed. The scheme of non-equilibrium charge carriers photogeneration process in these compositions is suggested.

Effect of molecular optical vibrations on thermoluminescence of silicon organic polymer

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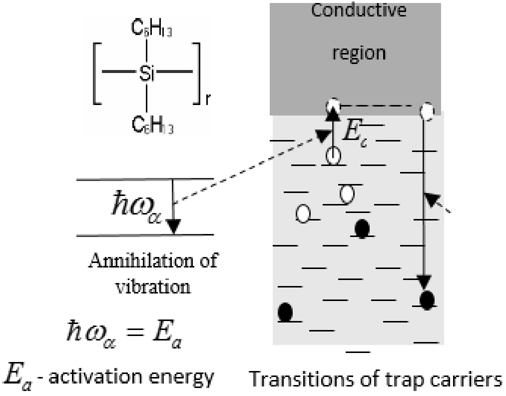
The suggested model describes the influence of optical vibration on termoluminescence of the systems with a quasi-continuous spectrum of traps [1]. The model is based on the fact that the thermal equilibration occurs after illumination much faster in the vibrational subsystem as compared to the electron level subsystem. The effects of transitions between the trapped charge carrier states accompanied by the disappearance of an optical vibration quantum on the thermoluminescence curve are investigated. It is shown that 1) the discrete set of the activation energies, which are equal to the optical quanta, should appear, though the trap spectrum is quasi-continuous, 2) the additional structure in TSL curve may arise. The dependence of manifestation of the effects on the system parameters is analyzed. The model explained the recently observed in [2] coincidence of the activation energies of charge carrier traps in thermoluminescence of a pure polymer poly(di-n-hexylsilane) with the energies of the vibrational modes seen in Raman spectra.



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[2] A.Gumenyuk, N.I. Ostapenko et.al. Chem. Phys. 394,(2012), 36.

Polymeric nanocomposites based on polytetrafluoroethylene and carbon nanotube: morphology and tribological properties

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Nanocomposites consisting of PTFE and carbon nanotubes (CNT) have been prepared and analyzed by the method of high resolution scanning electron microscopy (SEM). It was found that an addition of CNT dramatically changes the morphology of PTFE nanocomposites [1]. Morphology of initial samples was prose containing polycrysralline fibrillar lamellae and loose packing of structural elements. Adhesion of fillers to the matrix found to be weak with poorly resolved interface layer. The values of friction coefficients for nanocomposites with a different CNT content have been determined and their variations within a broad range (more than 70%) have been reported. It was shown that the intensity of linear wear diminishes for all PTFE-based nanocomposites with increasing CNT concentration in the range from 1% to 5% in 6 to 65 times from an initial value, respectively. It was established that modification of such composite caused by g-irradiation lead to significant changes in morphology and reduce linear wear correspondingly. Not irradiated samples originally exhibit a certain level of porosity, the presence of polycrystalline fibrilarlamels and low adhesion of filling material with matrix. Irradiation of CNT/PTFE composite at temperature above the melting point result in formation of spherolites, significant decrease in porosity and improved adhesion of filling material with matrix. Intensity of the linear wear down diminishes for all of composites of PTFE/CNT: with content 1,0; 2,5 and 5,0 % CNT in ~ $4\cdot10^3$; $2{,}5\cdot10^3$ and $3{,}5\cdot10^2$ times from an initial value, accordingly.

[1] Sadovskaya, N. V.; Sakhno, Yu. E.; Konova, E. M.; Sychkova, S. T.; Sakhno, T. V.; Khatipov, S. A. /Polymer Journal 2012, Vol. 34 Issue 4, p.353.

Intermolecular interactions in saccharide-water solutions under the influence of magnetic field

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The study of saccharides conformation change in liquid systems appears to be the serious problem related to the analysis of the neurochemical effects of interaction of biomolecules and bimolecular complexes [1]. In order to solve this problem, the investigations of magnetic field influence of liquid systems containing saccharides were carried out [2].

The specific conformational effects related to the formation of temporal concentration fluctuations during the process of mutarotation are distinctive for the regarded objects [1]. Light scattering in the glucose, lactose and sucrose - water solutions at the constant magnetic field of various inductions was investigated in the present work. The dependency of light-scattering intensity on the magnetic induction value was obtained. It led to the conclusion, that glycoside bond in sucrose prevents the formation of non-stable fluctuations of concentration in comparison with hydrogen bonds, which take part in the formation of the structures of this type in glucose and lactose solutions.

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[2] F. Lianes, C. Dias, D.H. Rayan, Magnetic Polysaccharides, International Journal of PolymericMaterials, 51:537-545, 2002

Spectroscopic investigation of the human leucocytes

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This work is part of the work, concerned with investigation of the spectral properties of human blood components - human leukocytes. The aim of the project is studying the spectra and identification the optical centers of absorption and emission. Measurements were carried out on the samples obtained from healthy donors and patients with chronic lymphocytic leukemia B, provided by [2]. Measurement of absorption was measured at room temperature, phosphorescence emission – at T = 78K. Results of the research shows, that in the spectra of leukocytes present limited number of centers, which belong to macromolecules, including areas of so-called conjugated bonds, both cyclical and linear. The main components that form the spectrum are peptides, nucleic acids (DNA, RNA), co-enzymes (NAD, NAD-H, NDAP, NAD-H). The comparison absorption spectra (Fig. 1) and low-temperature phosphorescence spectra (Fig. 2) lymphocytes from healthy donors and lymphocytes from patients shows significant differences.

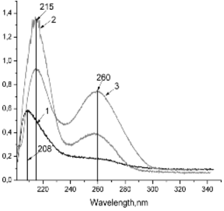

Fig.1 Absorption spectra: (1) – B- lymphocytes (normal), (2) – leukomass of a patient (leukemia B), (3) – RNA

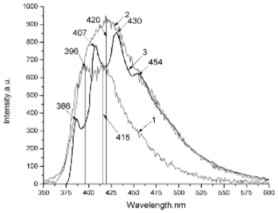

Fig.2 Phosphorescence spectra: (1) – B-lymphocytes (normal) T=78 K, (2) – leukomass of a patient (leukemia B) T=78 K, (3) – RNA T=4 K [1]

The absorption spectra of lymphocytes from patients have a characteristic broad absorption band with a maximum at 260 nm and healthy cells shows much weaker absorption band in this area, there is no maximum. In the region of 210 nm is also observed differences between the respective spectra [2]. Phosphorescence spectra from healthy donors and from patients also exhibit a fundamental difference: spectrum of healthy donors have two characteristic peaks (at 396 and 415 nm) spectrum of cells from patients - has a maximum at 425 nm and its overall shape is an envelope for RNA array [3]. We accume, that this difference shows a large amount of RNA that accumulates in cells with leukemia.

[1] Yashcuk V.M *et al.* Optical response of the Polinucleotid-proteins interaction // Mol. Cryst. Liq. Cryst., Vol. 535: pp. 93–110, 2011

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[3] O. M, Snitserova *et al.* Some peculiarities of the lymphocytes luminescence spectra // J. Bulletin of TSNUK. Series: Phys. & Math. – 2015. – N 1.

Luminescent characteristics of a number of new copolymers based on carbazole groups and lanthanoid (Eu, Tb)

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Nowadays organic luminescent materials spark a serious interest due to intense development of the organic- light-emitting diodes (OLED) and organic solar cells technologies. Such luminescent materials could potentially improve the color quality and efficiency of the organic light-emitting diodes, increase the efficiency of the electron-hole pairs forming in solar cells etc.

In this context copolymers with incorporated luminescent dyes are the subject of research interest both because it's ability to form homogenous polymer films, serving like polymer matrices for different luminescent dyes in particular, and because the ability of creating luminescence with specific color characteristics. Both these properties give such materials a research potential in the frame of OLEDs emission layers development.

In the present work spectral properties of a number of new copolymers on the base of carbazole groups and lanthanoid (Eu, Tb) were investigated. The copolymers showed good ability to form polymer films on its base and demonstrate excitation energy transfer from the carbazole groups to the lanthanoid molecules with corresponding photoluminescence in the green-red spectral region. However, for these compounds typical Eu and Tb photoluminescence is observing only in the solid state (film and bulk) while almost no such emission appears in the solutions.

Luminescence spectra of adenine molecules under the conditions of electrical discharge

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Information about the physical structure of molecules is necessary for understanding of the role of primary physical processes in ensuring the functioning of biological systems and for identification of the mechanisms of influence of the various environmental factors. The interaction of high-energy radiation with living cells, mostly does not lead directly to degradation of biopolymer molecules, this feature performs secondary electrons, which are produced in great quantity in biological matter.

This report refers to the experimental study of the luminescence phenomenon of the molecules adenine vapors in their excitation under the conditions of electrical discharge. The technique of the experiment is study optical spectra of electric discharge which light up the tube, filled with vapors of adenine molecules. The experimental layout consists of a discharge tube filled with vapors of the studied molecules, high voltage generator for discharge power, registration systems of the discharge radiation. Experimental conditions were as follows: pressure of molecules vapors ~ 10^{-2} Pa, the current intensity of discharge I = 10 mA, voltage in the discharge gap – 540 V.

During the research we have obtained phosphorescence spectra of discharge in the wavelengths region from 200 nm to 500 nm. Spectral bands with maxima at wavelengths of 284, 299, 312 − 315, 329, 337, 352 − 357, 373 – 395, 380 − 387, 400, 407, 417 − 424, 430, 436, 452 and 474 nm were detected in analyzing of these spectra. Some of these bands are absent in luminescence spectra of adenine initiated by electron beam [1].

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3

Computer Simulation

Symmetry reduction in ZnO magic clusters

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Discovery of ZnO magic clusters [1] in mass spectra of laser ablation of zinc peroxide bulk powder, initiated discussion on their structure. We suggest nested shell model to explain the observed magic numbers in the mass spectra. To validate the model, we performed a stress-test for the clusters: a small random displacement of all the atoms, and the following their geometry optimization. Multiple calculations have been run for statistical reasonableness of the results. The important option of the calculations was the possibility to keep a symmetry of a cluster during both the distortion and the geometry optimization. In such a way we have studied the total energy of the clusters on step-by-step reduced symmetry. It was found, that reducing the symmetry for some clusters lowers their total energy. The phenomenon may be explained by Jahn-Teller effect – symmetry reduction removes the degeneracy of the ground state, and thus lowers the total energy of the system [2].

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The study of metal-base pairing in DNA by means of Quantum Mechanics/Molecular Mechanics simulations

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The DNA molecule is an attractive material in pharmaceutical technology and nanotechnology. In the recent years there have been extensive interest for fluorescent, ligand-stabilized Ag_N–DNA systems [1-3]. The wide range of properties such as rich color palette, low toxicity, high fluorescence quantum yields of some clusters, low synthesis costs enabling many applications that employ Ag_N–DNA.

We focus on the stability determining factors of DNA–metal complexes, which are examined by performing all-atom molecular dynamics simulations and Car-Parrinello molecular dynamics/molecular mechanics (CPMD/MM) simulations. We highlight the importance of the argentophilic interactions in the geometry of the long metal-mediated strands and the role of hydrogen bonds for structure stabilization.

We use a parametrized 12-6 Lennard-Jones non-bonded model [4] for molecular dynamics step in order to describe the interaction between metal ion and nucleic acid in water environment.

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Vibrational spectra of salol and their interpretation on the basis of computer simulation

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IR spectra of salol have been measured in different phase states over a wide temperature range. The strongest difference between the IR spectra of different phases are observed in the spectral regions 1180-1240, 1650-1710, and 3000-3250 cm^{-1}. We suggest that conformational mobility of salol molecule and the influence of H-bonding are responsible for these differences.

Computer simulation of the conformers and dimmers have been performed using the DFT method with B3LYP/6-31 G(d) functional. Conformers, which we have simulated, differ from each other by the angle of rotation of one of the benzene ring relative to the other. Other geometrical parameters remained unchanged. H-complexes I and II are dimers with H-bonding between O-H groups, H-complex III is a dimer with H-bonding between O-H and C=O group.

Change in temperature causes a change in the conformational mixture and in the number of dimers. The dimers are formed by weak H-bonding.

In-plane stretching vibrations of C-O group and in-plane bending vibrations of the benzene ring in the spectral region 1180-1240 cm^{-1} undergo the most significant changes under conformational transitions. Changes of some vibrational modes in this frequency range are due to the dimerization of the sample.

The change of the shape of Q_R(C=O) in-plane stretching vibration band in the IR spectra in the spectral region 1650-1710 cm^{-1} in both crystalline phases is also associated with the formation of dimmers and conformational mobility. The presence of the intramolecular H-bonding between the benzene ring and C=O group of the salol molecule was established, a characteristic feature of which is a broad intense band C-H with a large width in the spectral range 3000-3100 cm^{-1}. The IR studies also indicate the presence of the intermolecular H-bonding, evidenced through large width of the υ (OH) band, its low frequency and high intensity.

Using the results of the simulations, IR spectra of salol were interpreted and the structure of salol in different phase states was presented.

Molecular modeling based by method of DFT and interpretation of IR spectra of 3’-bromobenzophenone

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Vibrational IR spectra of 3’-bromobenzophenone have been measured at 12, 297 and 365 K in the ranges 400-3200 cm^{-1}. Modeling of structure and vibrational spectra has been performed, by a density functional theory (DFT) method, is realized in a software package Gaussian’03. Functional B3LYP and Basis 6-31G(d) have been used for our calculations.

Energy, structure, dipole moment, polarizability, force constants, frequencies of normal modes in harmonic approximation and their intensities in the IR spectra have been calculated. Process of scaling has been used for decrease of the discrepancy between calculated frequencies in harmonic approximation and measured frequencies. Interpretation of IR absorption spectrum is given.

Nature of the Lowest Electron Transitions in Styryl Bases Bensothiazole Derivatives and Analogues Bearing Para- Methoxy and Trifluoromethyl Substituents in Phenylene Moiety

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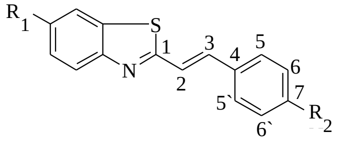
The results of both quantum-chemical and spectral investigation of dimethylamino-styryl bases of benzothiazole (BT) derivatives as well as their analogues with para- metoxy and -trifluoromethyl sybstityents at phenylene moiety are presented. Their formulae are presented in Figure.



R_1= H-, $(H_3C)_2N$- , H_3CO-

R_2 = $-N(CH_3)_2$, $-OCH_3$, $-CF_3$

UV-Vis absorption spectra were recorded on a Shimadzu UV-3100 spectrophotometer in toluene, acetonitrile (spectral grade). Quantum-chemical calculation of optimized molecular geometry were performed by HF/6-31(d,p) and DFT/CAM-B3LYP//6-31(d,p) methods; the electron transition characteristics were calculated by the non-empirical (TD/DFT/6-31G(d,p)/CAM-B3LYP) method and semi-empirical ZINDO method, using the package Gauss-03.

It was shown that going from cationic styryl/methoxy styryls to the corresponding neutral bases is accompanied by substantial change of the equilibrium molecular geometry and charge distribution at atoms, while absorbtion band undergoes the essential hypsochromical shift. It is established that introducing of the donor groups in the bases causes negligible change of the length of carbon-carbon bonds and the magnitude of atomic charges in the main chromophore, in contrast to the substantial changes of the magnitude and direction state dipole moments in both ground and excited states. The styryl bases bearing the donor groups in the benzthiazole moiety and acceptor p-CF_3 substituent at phenylene terminal group with the inverted direction of the dipole moment have been obtained. Spectral and quantum-chemical study have shown that some widening of the spectral bands is connected not with the second electron transition but with the vibronic interaction.

Simulation of the oxygen effect on the surface electronic structure for SnS and SnTe crystals

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The prediction of material surface properties variation under external conditions is very important in the development of opto-, micro- and nanoelectronic devices. Earlier we have studied the surface electronic structure for GeS and SnSe single crystals under the effect of oxygen and surface bending of energy bands for Sn-X (X= S, Se, Te) compounds [1-3]. In this work we focus on the analysis of oxygen atoms and molecules effect on the surface electronic structure for SnS and SnTe crystals.

The calculation has been based on the methods of linear combination of atomic orbitals and pseudopotential generalized in the works by W.A. Harrison [4]. The energy values have been determined in the Γ-point - the centre of the Brillouin zone. In construction of the energy band diagrams we used the atomic terms within Hartree-Fock approximation. Intratomic Coulomb repulsion energies and bond polarities have been accounted for. The following energy parameters have been computed: the valence-band maximum, the conduction-band minimum, the band gap, the Fermi level. Surface bending of the energy bands was determined as the difference between the energy of the surface states before the reconstruction and the Fermi level. The Fermi level was defined accounting for the position of the levels formed by the homopolar bonds, non-bonding and hybridized orbitals according to the procedure described in our work [1]. The correlation between the valence-band maximum and photoemission threshold, the band gap and optical band gap is considered.

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Phonon frequency calculations in $CaFe_2As_2$

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The discovery of superconductivity in Fe-based compounds with T_c in the range from 26 to 56 K has created a new paradigm in condensed matter physics. In the Fe-pnictide family, “122” compounds with AFe_2As_2 (A = Ca, Sr, Ba) are widely studied systems, where T_c can reach as high as 38 K [1]. In the “122” family, $CaFe_2As_2$ is found to be unique, where superconductivity emerges upon application of modest nonhydrostatic pressure. With hydrostatic pressure it undergoes a structural transition from a tetragonal phase to a collapsed tetragonal phase [2]. The collapsed tetragonal phase in $CaFe_2As_2$ is characterized by a ∼10% reduction in the c axis of the room temperature tetragonal phase. Magnetic and electronic structures are found to be strongly influenced by this transition.

We have carried out calculations of phonon spectra in the center of the Brillouin zone of this compound for both tetragonal and collapsed tetragonal phases. Our calculations have been performed within the density functional theory framework with a full-electron potential and an augmented plane-wave method with a local spin-density approximation – the program ELK [3]. The exchange-correlation potential was used in the form of a generalized gradient approximation (Perdew-Burke-Ernzerhof).

The results show that A_{1g} mode, corresponding to As atoms oscillations, has higher frequency (152.0 cm^{-1}, 177.1 cm^{-1}) than B_{1g} mode, corresponding to Fe atoms oscillations (162.4 cm^{-1}, 218.0 cm^{-1}). (But the mass of atom As is higher, than mass of Fe atom and the frequency of As mode should be less than the frequency of Fe). Furthermore, we have calculated electronic properties and phonon spectra for some fixed values of Fe spin moment. The magnetic moment varied from 1.65 μ_B to 2.3 μ_B. Phonon spectra demonstrate strong dependence from Fe magnetic moment.

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Kubelka–Munk theory application for random lasing modeling

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Kubelka-Munk theory (TKM) is commonly used to study of light reflection on the media with existing absorption and scattering. System of TKM equations describes the incoming flux falling on the sample, and the scattered flux moving opposite way. However, TKM may be extended to describe luminescence and lasing. We have modified TMK to study these media.

Pumping of scattering medium creates an active area with amplification (i. e. negative absorption coefficient), which can be represented as a separate sample. Lasing in the area appears due to luminescence throughout the active volume and moves amplifying by broken paths to exit of the active area. The maximum of lasing density is in the center of active area. Unlike the classic TKM, in our model the fluxes move not at the one (input) side, but at the both towards each other.

Taking into account the distribution of the path's lengths, and absorption and amplification coefficients depended on the lasing wavelength, allow us to obtain the spectral characteristics of the lasing. In particular, the spectrum's width and its energy density at the maximum can be used for detection transition of luminescence to lasing.

As results we obtained dependencies of luminescence and lasing fluxes' intensities distributed in the active area. Using that we found spectra parameters for different absorption and amplification coefficients, scattering centers concentration and, consequently, the fact of dominance of certain path lengths.

The results correlate with experimental data and allow us to determine parameters of the medium to provide transition to lasing, defined abrupt spectrum narrowing and step-like rising of energy density's maximum. As a conclusion we pointed that the described approach can be used for strongly scattering media modeling.

Optical trapping simulation of micron particles in Gaussian and Laguerre-Gaussian beams.

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Optical tweezers as an instrument of non-contact control of micro- and nano-objects gained widespread in various fields of science. They can hold, move, rotate, sort different types of particles using a focused laser beam. In this report the modeling of the forces acting on absorbing and metal particles was carried out with a T-matrix method.

There are many methods that are used to simulate the interaction of light and small particles. Notable ones: DDA [1], VIEM [2], FDTD [3] are tedious and require considerable calculations. The T-matrix [4] is the most convenient method in this class. It’s based on decomposition of incident, passed and scattered fields in a series of spherical vector wave functions.

Optical Tweezer Toolbox [5] was used to calculate the radiation and scattering forces acting on the particles under different conditions. It was shown that in the ordinary Gaussian beam the metal particle (Au, n=0,86+1,85i, r=2λ) is pushed out of the trap in both radial and azimuthal directions. If we take Laguerre-Gaussian mode LG_0^1 the particle is held in the center of the beam in the area with a minimum intensity; concurrently the capture in the longitudinal direction is unstable. Taking into account the mass of the particle, it becomes possible to create an effective three-dimensional trap.

Note that existence of the optical trap depends on the ratio between the beam waist and the particle size. For particles whose diameter is less than the laser wavelength it is possible to make a trap with a conventional Gaussian beam. In addition, there are two modes strongly dependent on the particle size. In one mode the particle escaped from the trap at the other attracted. Therefore, all the factors that have an effect on the stability of the capture must be taken into account.

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Simulation of quartz nanocrystals cracking by molecular dynamics method

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It is well known that shortly before and during earthquake some electromagnetic radiation emission from the earth's crust bowels can be detected above seismic disaster array up to satellite orbits. This can be explained due to presence of quartz crystals in the Earth's crust which have very pronounced piezoelectric properties, all the more so the mass fraction of SiO_2 in the crust is about 50%. The researches [1, 2] have confirmed this assumption but were performed within the continuous medium model together with specified crack dynamics. However, applicability of this model for nanoscopic quartz crystals with structural defects under influence of ruinous stresses currently remains open.

In the article the computer simulation of small size crystal destruction was performed, cracking of quartz nanocrystals were explored and obtained results were compared with [1, 2]. Calculations were carried out by molecular dynamics method for the SiO_2 crystal with 4128 atoms using several interatomic potentials [3, 4] which take into account piezoeffect in different approximations. Obtained results for both potentials are partially agreed with obtained in [1, 2], namely: new formed surfaces of crack near its apex is approximated by a parabola with the smallest deviation; separate groups of atoms are inside of crack sometimes linked to its surfaces; value of total dipole moment p of nanocrystal during of its breaking has oscillations, period of whose is close to the time required for acoustic wave to ensure that passed through the crystal – Fig. 1.

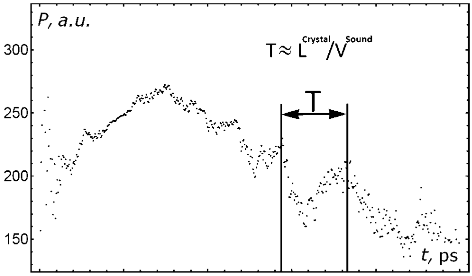

Fig. 1. The time-dependence of crystal dipole moment during its rupture.

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4

Crystals

Crystallographic basis of phase transformation in shape memory alloys

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Shape memory effect is a peculiar property exhibited by a series of alloy systems. These alloys are temperature sensitive materials, and their crystal structures change in a certain temperature interval, on cooling and heating by means of martensitic transformation and reverse transformation, respectively. Martensitic transformation is a displacive phase transformation and occurs in the materials on cooling from high temperature parent phase region. These alloys have an ability to recover the original shape on heating after deformation in low temperature product phase condition in bulk level. Shape memory effect is facilitated by martensitic transformation governed by changes in the crystalline structure of the material in the crystal and lattice level. Martensitic transformations occur with the cooperative movement of atoms in two opposite directions, <110 > -type directions on the {110}-type planes of austenite matrix.

Thermal induced martensite occurs as lattice twinning by means of lattice invariant shear, and the twinned martensite structures turn into detwinned structures by means of reorientation of twinned martensite with deformation of the material in the martensitic condition. The deformed material recovers the original shape on heating, and cycles between the deformed and original shapes on cooling and heating, respectively. Meanwhile, the parent phase structure returns to the detwinned structure on cooling, and the crystal structure of material cycles between the ordered parent phase structure and detwinned martensite structure on heating and cooling.

Copper based alloys exhibit this property in metastable β-phase region, which has bcc-based structures at high temperature parent phase field, and these structures martensiticaly turn into layered complex structures with lattice twinning process on cooling. Lattice invariant shear is not uniform in copper based shape memory alloys, and these shears gives rise to the formation of layered structures, like 3R, 9R or 18R depending on the stacking sequences on the close-packed planes of the ordered lattice.

In the present contribution, X-ray diffraction, transmission electron microscopy (TEM) and differential scanning calorimetry (DSC) studies were carried out on two copper based CuZnAl and CuAlMn alloys.

Excitation energy transfer mechanisms in $M^{II}MoO_4$ molybdate crystals

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Despite intensive research efforts, the mechanisms of the excitation energy transfer in processes of intrinsic photoluminescence (PL) in $AMoO_4$ molybdates are still the subject of discussion [1]. In particular, the role of free charge carriers at the stages of PL excitation and the excitation energy transfer to PL emission centers has not been clarified up to now. An open question is what peculiarities of intrinsic PL excitation spectra of $AMoO_4$ molybdates imply participation of free charge carriers, and what spectral details should be attributed to intra-center excitations of the luminescence centers without generation of such carriers at any stage of PL processes. As the key point that can enable solution of this problem, we regard studies of the properties of the crystals which provide information on the spectral threshold of generation of free charge carriers. Such properties are in particular, the dependencies of photoconductivity and thermo-stimulated luminescence (TSL) intensity on the incident photon energy.

The systematic studies of the PL excitation spectra, photoconductivity and TSL dependencies on incident photons energy are presented in this work for the set of molybdates with various cations (Ca, Sr, Zn, Cd, Pb). Experimental results are analyzed together with results of the first-principles calculations of their electronic structures. The electronic band structures of studied crystals were calculated by the FP-LAPW method [2]. The effective masses of electrons and holes at the band edges of the crystals are estimated within parabolic approximation of the energy dispersion curves. The origin of the free charge carrier excitation threshold and peculiarities of the PL excitation spectra in studied compounds are clarified using the electronic structure results.

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Crystal structure, vibrational spectra and DFT modeling studies of melaminium n-acetylglycinate dihydrate

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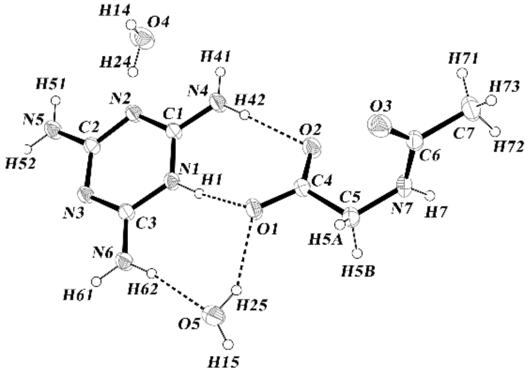
The new crystal was obtained in reaction of melamine and N-acetylglycine in the water solution. Melaminium N-acetylglycinate dihydrate crystallizes in triclinic system, in P-1 space group. The lattice constants at room temperature are: a=5.642(1), b=7.773(2), c=15.775(3) Å, α=77.28(1), β=84.00(1), γ=73.43(1) °, V=646.2 Å3, Z=2. The asymmetric unit comprises one monoprotonated melaminium cation, one N-acetylglycinate anion and two water molecules. The structure is stabilized by N−H···O, N−H···N and O−H···O hydrogen bonds. The NBO analysis has revealed that the n(O1)→σ(N1-H1) interaction gives the strongest stabilization to the system. In the crystal structure of studied compound, chain patterns of hydrogen bond occur in *ab* plane. Two chains propagate along main crystallographic directions *–a,b*. They are created without the melaminium cations. The cations form chain patterns exclusively along [110] direction.

The IR and Raman spectra were obtained for the protonated and deuterated crystals. The vibrational spectra were interpreted by using PEDs (Potential Energy Distributions). The theoretical and observed frequencies have been compared and several stretching and deformation modes confirm the presence of intermolecular hydrogen bonding in the title crystal.



The frontier molecular orbitals show that the stability of the title compound increases in going from the gas phase to the solution phase.

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The origin of luminescence centers in CeO_2 nanocrystals

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Cerium dioxide CeO_2 is widely used in many technical applications such as catalysis, gas sensors, electrochromic and UV coatings, etc. At last time, many researches focused on nanocrystalline CeO_2 due to possible applications in the field of electroluminescent devices, integrated optics and in biomedicine [1]. Nanocrystalline ceria possess strong antioxidative activity associated with reversible $Ce^{4+} \leftrightarrow Ce^{3+}$ reduction/oxidation processes facilitated by high degree of oxygen non-stoichiometry of CeO_{2-x} nanocrystals [2-3]. Luminescence of CeO_2 is usually assigned to crystal lattice defects formed by oxygen vacancies, but the obvious experimental evidences of this assumption are absent. We have clarified the nature of luminescence in stoichiometric and oxygen-deficient CeO_2 nanocrystals and determined the microscopic feature of Ce^{3+} luminescent centres.

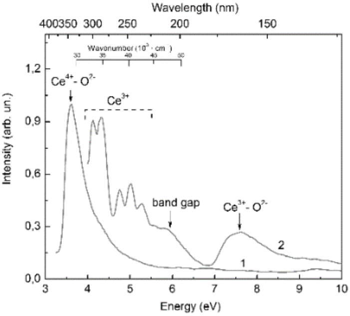

Fig.1. Excitation spectra of oxygen-deficient CeO_{2-x} nanocrystals at T=10K, 1–λ_{reg}=630 nm, 2–λ_{reg}=390 nm.

CeO_2 powders were synthesized by Pechini citrate gel method. To determine whether the luminescence of CeO_2 is related to oxygen vacancies, the nanocrystals were annealed during 2 h in different atmospheres – oxidative (air), neutral (argon) and reducing (hydrogen) at 1000°C. Luminescent properties have been investigated at SUPERLUMI setup (DESY) in Hamburg, Germany using synchrotron radiation.

It has been found, that luminescence of nanocrystalline ceria is not assigned to oxygen defects, but it is caused by the radiative relaxation in two types of optical centres, namely, Ce^{4+}-O^{2-} charge transfer state (λ_{max}= 630 nm) and Ce^{3+} ions, stabilized by oxygen vacancies (λ_{max}= 390 nm). Analysis of splitting of the Ce^{3+} excitation bands has shown that oxygen vacancies are formed at the nearest-neighbor position to the cerium ion. The ratio of Ce^{4+}/Ce^{3+} centres has been shown to be strongly depended on the amount of oxygen vacancies. Therefore, the increasing non-stoichiometry of ceria nanocrystals leads to the enhancement of Ce^{3+} luminescence. So, the changes in cerium luminescence signal as a result of $Ce^{3+} \leftrightarrow Ce^{4+}$ reactions observed, for instance, in living organism and associated with ceria biological activity could be the tool to visualize and trace such redox processes.

The investigations with synchrotron radiation at the SUPERLUMI station were performed in the frame of the I-20110938EC and NCN Polish No. 2012/07/B/ST5/02376 research projects.

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The plurality in the unity.
What do we know about guanidinium nitrobenzoate crystals?

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The crystallographic structures of guanidinium 4-nitrobenzoate and guanidinium 3-nitrobenzoate salts are known in literature. According to x-ray crystallographic study performed by Adams and co. [1] guanidinium 4-nitrobenzoate crystal belongs to monoclinic system with space group: $P2_1$ or $P2_1/m$. The additional research shown [2] that this crystal is noncetrosymmetric and belongs to $P2_1/m$ space group. Extended investigations made by Arumanayagam and Murugakoothan [3] indicate that this crystal has NLO properties. The SHG behavior was confirmed by Kurtz-Perry technique. The NLO signal is ca. 3-times stronger than that noticed in the case of KDP standard. On the other hand, the deeper studies of electronic structure, some vibrational properties and intervening orbital interaction were studied recently by Sasikala and co. [4]. Additionally, our DSC and low temperature infrared spectra investigations prove the continuous phase transition at ca. 180 K.

Surprisingly, investigation of guanidinium 3-nitrobenzoate compound shown that this crystal belongs to $P2_12_12_1$ space group of orthorhombic system [5]. The macroscopic inversion center in this space group is absent. That is way this compound can be used in NLO, but literature data are not available. Our TD-HF calculations show unambiguously that this compound can be used as SHG generator.

In the literature 2-nitrobenzoate guanidinium is not known. It is possible to obtain this crystal? And what space group will be realized in this compound? The presented DFT calcualtion and experiemtnal data can help in these answers.

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Peculiarities of self-trapped excitons luminescence from rare-gas cryocrystals under selective photoexcitation at the edge of exciton absorption

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The most prominent feature in luminescence of Xe, Kr and Ar – the so-called *M*-band – is formed by $^{1,3}\Sigma_u^+\rightarrow{}^1\Sigma_g^+$ transitions in (R_2*) excimer-like molecular self-trapped excitons (M-STE). The analysis of the luminescence spectra of rare-gas cryocrystals under different excitation conditions, excitation energies and crystal-growth conditions made it possible to elucidate the internal structure of *M*-bands. Each of the *M*-bands can be well approximated by two Gaussians: low energy 'defect' subband M_1 and high energy one M_2 which is dominant in the luminescence of more perfect samples. The threshold energies E_1 and E_2 for the M_1 and M_2 subbands excitations below the $n=1$ exciton energy were determined [1], but in the range $E_1<E<E_2$ of photon excitation energies there was no reproducibility in M_1-band spectral position and it was necessary to vary it during deconvolution of the luminescence spectra of rare-gas cryocrystals.

In the present paper we compare the luminescence of self-trapped excitons at selective photon excitation below and above the threshold energy E_2 of the samples of solid Xe, Kr and Ar. The experiments were performed at the SUPERLUMI experimental station at HASYLAB, DESY, Hamburg [2]. In the case of solid Xe and Kr at photon excitation in the range $E_1<E<E_2$ the *M*-bands may be well approximated by single Gaussian with spectroscopic parameters – (band position; FWHM, in eV) – *M'*(7.023;0.204) for Xe and *M'*(8.29;0.252) for Kr. In some cases the existence of additional subband *M'* was necessary to take into account during spectra deconvolution. In solid Ar the presence of additional band *M'*(9.4;0.3) was detected in all range $E_1<E<E_g$ of photon excitation, but, contrary to the case of solid Xe and Kr, there was no photon excitation energy at which the subband *M'* was in the M-STE spectrum alone. Nevertheless, a considerable part of the M-STE emission from solid Ar may be attributed to subband *M'*. Formation *M'*-emitted centers may be attributed to the trapped molecular center creation as a result of formation of nucleation states due to thermal lattice disorder in the ground state [3], which intensifies near the lattice defects and direct photoabsorption by such centers results in *M'*-band emission.

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Crystal structure, electronic band structure and luminescence of ZrO_2:F and ZrO_2:F,Eu crystals

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Doping of oxide materials is widely used in order to improve their optical, in particular luminescence properties. There are two possible ways to do such doping – by introduction of impurities in cationic or anionic position in crystal lattice. While the effects of the rare earth ions on characteristics of oxide compounds had been studied intensively during last decades, very limited data on impact of anion substitution on luminescent and scintillation characteristics of oxide materials are available at present. The number of reports about excellent optical, electrical and magnetic properties of the oxyfluoride and oxynitride compounds was published recently but knowledge about physical processes in such materials is very limited due to the lack of experimental and theoretical data [1, 2]. In this work the results of experimental and theoretical studies of fluorine-doped zirconia have been combined in order to clarify understanding of physical processes in anion-substituted materials.

The set of solid solutions of ZrO_2:F with fluorine content 2–20 mol.% has been prepared by solid state technique at 1000°C . The samples have been studied by powder XRD, SEM imaging and luminescence spectroscopy. For structural change analysis by luminescence spectroscopy the samples were doped with 0.5 mol.% of Eu^{3+}.

The crystal and electronic band structure calculations with geometry optimization have been carried out for a set of ZrO_2 crystals doped with fluorine and europium.

We have shown that substitution of fluorine in anionic sublattice leads to vacancies formation and deformation of main structural units of oxide compounds. Analysis of electronic structure fluorine-doped oxide compounds shows that ions F^- do not participate directly in electronic transitions.

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Photorefractive parameters of the doped $Sn_2P_2S_6$ ferroelectrics crystals

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The $Sn_2P_2S_6$ crystals are known as promising photorefractive materials for red and near infra-red spectral range with high amplitude parameters and fast enough response time, possessing a great perspectives of applications in red and near infrared spectra range. It was shown by previous works that an enhancement of the optical, photorefractive and dielectric properties of these materials can be achieved by variation of the growth technology and by goaled doping with Te, Sb, Bi [1]. In the communication we present new experimental data on the photorefractive parameters of the $Sn_2P_2S_6$ crystals, modified by goaled doping with Fe, In, Mn, and Cu during the growth using vapor-transport method. The basic photorefractive parameters, namely the photorefractive two-wave mixing gain and the response time, are measured using conventional holographic technique at 633 nm laser wavelength. Besides, first-principle model calculations of the electron spectra of these impurity states in the $Sn_2P_2S_6$ matrix were performed. It was shown that doping by the various metals with unfilled 3*d*-shells creates the additional donor levels in the gap, that enhances the electron component of the conducticity and so leads to increased electron-hole competition at the photorefractive grating formation. The possible models of these defects and perspectives of the further modifications of the $Sn_2P_2S_6$ crystals are discussed.

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Symmetry and electronic spectra of impurity in molecular crystals

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Most of the compounds used as impurity agents are derived from highly symmetrical molecules (naphthalene, anthracene, pyrene, etc.). Such molecules provide the basis for the formation of an entire class of organic compounds by means of substitution of one or several atoms of hydrogen with heteroatoms. If the equivalent atoms present in the highly symmetrical molecules are substituted, it is possible to form the isomer molecules. So, for instance, if a hydrogen atom is substituted with a heteroatom in one of the four equivalent positions 1, 5, 4, or 8 in a naphthalene molecule, it leads to the formation of four isomeric molecules.

Previously it was shown [1], that monosubstituted derivatives of naphthalene dissolved in crystalline naphthalene generate impurity centers of two types, which are represented in the low-temperature absorption and fluorescence spectra by two identical series of spectral bands. The aim of the present work is to study in detail the low-temperature luminescence spectra of naphthalene doped with its dichlorosubstituted derivatives.

Two chlorine atoms in the 1,5-position for naphthalene under the influence of group symmetry operators for the free molecule D_{2h} and the crystal C^5_{2h} transforms into other equivalent position 4,8. The low-temperature luminescence spectrum of 1,5-dichloronaphthalene in naphthalene consists of two identical series of bands with initial bands at ν_{01}=20 098 cm^{-1} and ν_{02} =20 087 cm^{-1} (phosphorescence), ν_{01} = 30 466 cm^{-1} and ν_{02} = 30 096 cm^{-1} (fluorescence).

A symmetry group-theory analysis shows that for 2,3–dicloronaphthalene dissolved in a naphthalene crystal, a single impurity center is generated.

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Synergetic effects at the temperature phase transitions in long-chain aliphatic condensed compounds

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In the present work we report on FTIR spectroscopy and differential calorimetric studies of n-alkanes C_nH_{2n+2}, n-carboxylic acids $CH_3(CH_2)_{n-2}COOH$, cholesteryl myristate ($CholC_{14}$) and cetyltrimethylammonium bromide (CTAB) crystals in the temperature range from 100 K to the crystal melting point. The peculiarities of the molecular conformation, libration motions and other arrangement at the first-order phase transitions in these materials in different crystalline phases are investigated.

Also the theory of resonance dynamic intermolecular interaction of vibrations at such phase transitions is developed. In the framework of statistic and dynamic models, different mechanisms for the temperature changes in the Davydov’s splitting value of vibrational modes in the title crystals are investigated. It is shown that in addition to thermal expansion of crystals under heating, the damping of vibrational excitons on orientational and positional defects of different nature takes place. Theoretical analysis and computer simulation of resonance dynamical intermolecular interaction effect on the intramolecular vibrations spectra of the long-chain aliphatic crystals are carried out in terms of stochastic equations with account of different mechanisms. Good agreement between the experimental and computer simulation results was obtained.

Transition of natural zircon from crystalline state to the nanoparticles

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Zircon is a mineral single crystalline phase formed in the ZrO_2-SiO_2. This mineral, as well as other minerals in which metamict state is fixed, is able to maintain the appearance of crystalline material and still have an amorphous structure. During metamictization, zircon changes its physical and chemical properties. Metamict minerals has been studied in a large number of works, both experimental and theoretical [1]. Metamict zircon consists of amorphous SiO_2, and amorphous or microcrystalline phase ZrO_2. This mineral has at least three steps: crystalline zircon, zircon intermediate (composed of crystalline phase and partly solid phases of oxides ZrO_2, SiO_2) and zircon metamict.

In this report, 3 stages of geological development of zircons are studied with electron paramagnetic resonance (EPR). Metamictization of mineral has been monitored by X-ray method.

With EPR method, a set of electron-hole centers were obtained for zircon crystal that are well described in the literature [2]: SiO_4^{5-}, SiO_3^{3-} and SiO_2^{-}. The collection of intermediate zircons has centers of crystalline zircon and a set of EPR centers characteristic of amorphous SiO_2. These are the centers of quartz type: D-center O_2^{3-} with compensators (H^+ and Li^+). In addition to these centers, the SiO_4^{5-}, SiO_3^{3-} centers of zircon crystalline phase were observed. The fully metamict zircon is characterised by centers of "quartz" type and E_1'. The EPR spectra of these centers were broadened in comparison with the spectra of quartz. Metamict zircons were controlled by X-ray diffraction, and the size of crystallites in metamict zircon ranged from 145 to $85x10^{-1}$ nm. In natural zircon samples the process of transition to the level of crystal nanoparticles has been observed. From the above it may be concluded that the degree of crystallinity and an amorphous phase in zircons can be monitored by EPR method.

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Phonon and magnon Raman scattering in $LiNiPO_4$ single crystal

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$LiNiPO_4$ is an isolator belonging to the olivine family of lithium orthophosphates $LiMPO_4$ (M=Mn, Fe, Co and Ni) with space group *Pnma* (z=4). All member of this family were found to be antiferromagnets (AFM) with the same magnetic structure differing only in the spin-direction. These insulators exhibit strong linear magneto-electric (ME) effect in the AFM state. Ferroelectricity is generated by the long-range magnetic order being perturbed by the magnetic field. $LiNiPO_4$ undergoes magnetic transition at T_N = 20.8 K. Main features of the ME effect in $LiNiPO_4$ can be explained by connections between super-exchange, Dzyaloshinsky-Moriya interaction and elastic distortions (a uniform displacement of the PO_4 tetrahedrons along a-axis) [1].

The Raman spectra of a single crystal of $LiNiPO_4$ for a wide temperature range 2-300 K are reported. Of the 36 Raman-active modes predicted by group theory, 33 have been detected. The internal-external modes approximation is satisfactory by comparison of Raman data for $LiNiPO_4$ [2] and $LiCoPO_4$ [3]. The frequencies of translational vibrations of tetrahedrons PO_4 have been defined by comparing the experimental data with results of a computational simulation for the olivine $LiMPO_4$ (M = Co and Ni) [4].

In the AFM phase new features are observed in the low-frequency Raman spectra. Well below T_N the *YY* spectrum comprises a sharp peak at 60 cm^{-1}, accompanied by a broad asymmetric band with a maximum intensity at 66.5 cm^{-1}, and the cutoff frequency is about 120 cm^{-1}. There are peaks at 58.5 cm^{-1} in the *ZY* spectrum and at 50 cm^{-1} and 56.5 cm^{-1} in the *XY* spectrum. The observed peaks are attributed to magnon scattering, because they vanish above T_N. The origin of these magnetic excitations is discussed in comparing with the data of the neutron scattering investigations [1].

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Lattice dynamics of $CdWO_4$

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The first-principle calculations are employed to study lattice dynamics of cadmium tungstate. The equilibrium structure of wolframite-type crystal and lattice vibrations were calculated within the density functional theory using CRYSTAL09 program. The hybrid B3LYP exchange-correlation functional was used.

Cadmium tungstate has wolframite-type structure with monoclinic crystal lattice. The space group of $CdWO_4$ is P2/c (C^4_{2h}). In this structure each W atom is surrounded by 6 near O atoms in approximately octahedral coordination.

Group-theoretical analysis of the wolframite structures with C^4_{2h}(P2/c) space group gives the irreducible representations of vibrations as $\Gamma = 8Ag+10Bg+7Au+8Bu$, where Ag and Bg are Raman active, while Au and Bu are infrared active.

The vibrational modes of $CdWO_4$ were calculated theoretically and determined experimentally by Raman and IR reflection spectroscopy.

The number of Ag and Bg Raman active vibrations exactly corresponds to the number determined on the basis of group-theoretical calculations.

Spectroscopic and thermal characterization of novel catanionic surfactant complexes for advanced applications

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During the last decades, catanionic surfactants (CAS), which are a mixture of cationic and anionic surfactants, are attracting much interest both from fundamental (crystal engineering and supramolecule development) and applied point of view. The CAS compounds are of great application potential as lubricants and detergents in industry and technology, as well as for various encapsulation and controlled-delivery processes in pharmacy, medicine, and biology. Structure, morphology and properties of CAs depend on many factors, including properties of initial surfactants, their molar ratio, type of solvent and others. The primary aim of the present study is the investigation of the crystal structure and thermal properties of the solid phase CAS built of a carboxylic acid $CH_3(CH_2)_nCOOH$ (n=12, 16, 22) as anionic surfactant, and a cationic surfactant cetyltrimethylammonium bromide (CTAB), $[H_3C\text{-}(CH_2)_{15}\text{-}N^+(CH_3)_3]^+Br^-$, which are of particular interest as novel promising CAS. The prepared complexes were characterized using X-ray diffraction, differential scanning calorimetry (DSC), and temperature-dependent FTIR spectroscopy. It was shown, that supramolecular structure is formed, that consists from $CH_3(CH_2)_nCOO^-$ and $[H_3C\text{-}(CH_2)_{15}\text{-}N^+(CH_3)_3]^+$ parts which are held together by both hydrogen bonding and electrostatic interactions. This is confirmed with the experimental vibrational spectra. All the prepared CAS crystals have a bilayer structure. When following the thermotropic behaviour, the break up of the CAS complex is observed along with various disordering and melting transitions of the alkyl chain tail. By systematically varying the length of the alkyl radical of the CAS complex, we hope to shed some light on the structure of the complexe itself and in particular carboxylate bonding modes.

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Optical and dielectric parameters of the modified $Sn_2P_2S_6$ ferroelectrics

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The $Sn_2P_2S_6$ crystals are proper ferroelectrics with second-order phase transitions at $T_0 = 337$ K, and are known as promising piezoelectric, pyroelectric and photorefractive materials. Their potential applications require a search of the efficient ways for modifications of the key material parameters. The modifications can be realized by doping during the sample growth, and also at their post-growth treatment by sample annealing and indiffusion of the foreign elements from the surface layers. In this work we present results of the comparative studies of the optical, photorefractive and dielectric parameters, obtained with the $Sn_2P_2S_6$ crystals doped by Ag, Cu an Mn incorporated at their growth and by indiffusion into crystalline plates with different orientation. The optimal regimes of the indiffusion processes were found by varying the annealing temperature and time, and optimal conditions were determined. The measurements show that these various defects substantially change the dielectric and optical parameters, and the variations occur not only with values but also with anisotropy of the dielectric permittivity, that was measured on the orthogonal cuts of the modified samples. The optical transmission of these samples is strongly modified by indiffusion, whereas the samples doped with the same elements at growth do not change the optical transmission. An impact of the doping and indiffusion on the photorefractive parameters manifest itself as an increasing of the compensative component of the space-charge grating. The obtained experimental data correlate well with the results of the first-principle electron spectra modeling in various atom substitutions and positions of the defects.

Spectral investigation of the crystals and solutions of chelate zinc complexes with sulphanylaminosubstituted benzothiazoles

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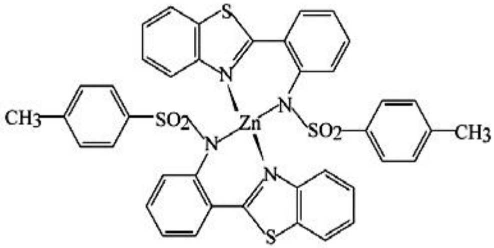
Zinc chelate complex with sulphanylaminosubstituted benzothiazoles ($Zn(TSA\text{-}BTZ)_2$) are perspective materials for organic light emitting devices (OLED).

In the process of electric and photo-radiation the same electronic states of molecules are involved, which leads to the similarity of the spectra of electroluminescence and photoluminescence. To study these processes the present work provides for a comparative spectral research of solution, polycrystalline powder and crystals of $Zn(TSA\text{-}BTZ)_2$, which structural formula is shown in Fig.

The powder $Zn(TSA\text{-}BTZ)_2$ is of a white colour, highly soluble (1 mg/ml) in acetonitrile and dimethyl sulfoxide. $Zn(TSA\text{-}BTZ)_2$ crystals were obtained by evaporation of the solution in acetonitrile. Solutions substances in organic solvents as well as crystals are transparent and have no absorption bands in the visible area of the spectrum.



On photoexcitation (with λ~365 nm), all samples have intensive luminescence. A luminescence of solutions and polycrystalline powder $Zn(TSA\text{-}BTZ)_2$ has bluish color, a single structureless band with peak λ~465 nm is observed in the spectra. The results are well corresponding with prior studies of $Zn(TSA\text{-}BTZ)_2$ electroluminescence spectra and allowing to identify this luminescence as its own zinc complex luminescence.

The luminescence of crystals $Zn(TSA\text{-}BTZ)_2$ differs significantly from luminescence of solutions and polycrystalline powder. The luminescence is of a bright yellow colour, the maximum of photoluminescence band is shifted to long-wave area and counts λmax ~ 520 nm. This luminescence was not observed in the spectra of electroluminescence and comparative analysis of the $Zn(TSA\text{-}BTZ)_2$ spectra in various states of aggregation to determine the excimer nature of the luminescence.

Spectroscopic studies $K_3Bi_5(PO_4)_6$, $K_2Bi(PO_4)(MoO_4)$ and $K_5Bi(MoO_4)_4$ crystals doped with rare-earth ions

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The Bi-containing oxide crystals are considered as perspective hosts for luminescent rare-earth (RE) ions since the Bi^{3+} ionic radius is close to ionic radii of the lanthanides. The photo-luminescence (PL) properties of the RE-doped Bi-containing phosphates and molybdates are intensively studied from viewpoint of practical applications, namely as effective components of white light emission diodes, promising phosphor and laser host materials [1]. In this work we present the results of spectroscopic studies of a set of newly-synthesized Ln-doped Bi-containing crystals. These results are analyzed in the context of potential of the studied compounds as novel luminophores for various applications.

The polycrystalline samples of $K_3Bi_5(PO_4)_6$, $K_2Bi(PO_4)(MoO_4)$ and $K_5Bi(MoO_4)_4$ doped with several types of RE ions (Eu, Tb, Pr, Tm, Ce) were synthesized by spontaneous crystallization method. The luminescence spectroscopy studies were carried out under the VUV synchrotron excitations in 4-25 eV region of excitation energies. The temperature dependencies of the luminescence properties under nitrogen laser and xenon lamp excitations were investigated in 4.2-300 K temperature range. Diffuse reflectance spectra of the samples were measured at 300 K using double-beam SPECORD M40 spectrophotometer.

The studied crystals reveal intensive RE^{3+}-related emission lines under excitations with photon energies in the UV and VUV regions. In some cases, these bands are accompanied by wide bands of intrinsic PL of the hosts. The PL excitation spectra of the studied RE-doped samples reveal excitation bands formed by the host excitations even when registered in emission bands of corresponding RE^{3+} ions. Formation of the PL excitation spectra of studied compounds are analyzed from viewpoint of contributions from the host-related transitions and the charge-transfer bands of RE^{3+}. Attribution of the RE-related PL emission bands is done.

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Optical properties of $PbGa_2S_4$ crystal

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The high-frequency refractive index of $PbGa_2S_4$ crystal has been calculated using the Harrison bonding-orbital method [1, 2].

Proceeding from the structure of electron shells of the atoms forming a $PbGa_2S_4$ crystal, one can conclude the following. Lead atoms are divalent, and electrons of these atoms are located in the outer shells in the *p*-state. Gallium atoms are trivalent. In this case, one electron in the outer shell is in the *p*-state, while the two others are in the *s*-state. When a bond is formed, one electron passes from the *s*-state to the *p*-state. Finally, sulfur atoms have two electrons in the *p*-state in their outer valence shells. Thus, the binding energies between *p* states make the dominant contribution to the crystal properties.

The crystal properties are studied using the calculated energy of the covalent bond V_2 and ionic bond V_3. Energy V_2 is determined by the interaction between the electronic states of atoms (for example, the *s*-state of cation and the *p*-state of anion), while energy V_3 is determined by the difference between the Hartree–Fock single-electron energies, $\varepsilon_s - \varepsilon_p$. Table 1 contains the Hartree–Fock energies for the atoms forming the $PbGa_2S_4$ crystal [2]. The calculation results are listed in Table 2.

Table 1. Hartree–Fock energies (in electronvolts) for valence electrons

Energy	Pb	Ga	S
ε_s, eV	-12.49	-11.55	-24.02
ε_p, eV	-6.53	-5.67	-11.60

Table 2. Calculated characteristics of $PbGa_2S_4$ crystal

Bond type	N_c	d, Å	V_2, eV	V_3, eV	α, Å^3	χ	γ
Pb-S	8	3.03	3.24	2.53	16.01	0.072	0.75
Ga-S	4	2.32	3.92	2.96	17.11	0.172	1.5

Having determined polarizability and, then, susceptibility χ of $PbGa_2S_4$ crystal, one can find the refractive index as $n^2 = 1 + 4\pi\chi$. Thus, $n_{\text{theor}} = 2.02$. The ratio of the calculated value n_{theor} to the experimental value ($n_{\text{exp}} = 2.51$) is 0.8; this is quite satisfactory agreement, with allowance for the fact that the $PbGa_2S_4$ unit cell contains 224 atoms.

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Influence of molecular geometry of cyclic hydrocarbons on the isochoric thermal conductivity

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This work presents the results of study of the mechanisms of heat transfer in molecular crystals in orientationally disordered phases of cyclopentane C_5H_{10} and cyclohexene C_6H_{10}.

Orientationally disordered phases of cyclic hydrocarbons with different geometry of molecules have been investigated for the first time, and it was shown that thermal conductivity increases with temperature. This behavior can be attributed to the attenuation of phonon scattering at short-range orientation order fluctuations.

A comparative analysis of the temperature dependences of thermal conductivity of the investigated compounds C_5H_{10}, C_6H_{10} is made jointly with previously studied benzene C_6H_6 and cyclohexane C_6H_{12}. It is shown that the thermal conductivity varies in different compounds depending on the geometry of the molecule.

The results of the present study confirm the conclusion that disinhibition of uniaxial rotation of molecules like a disinhibition of rotation of the molecule as a whole, leads to an increase in isochoric thermal conductivity with increasing temperature.

Features of the electronic structure of calcium apatites

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Electronic structure of calcium apatites $Ca_{10}(ZO_4)_6X_2$, where Z=P, As, V; X=OH, F, Cl, was investigated with spectral methods and quantum-mechanical modelling in LMTO-approximation. Determinate role of tetrahedral oxygen matrixes XO_4^{3-} in the formation of the main features of a valence band of the studied structures is shown.

It is established that the electronic structure of stochiometric apatites is low-sensitive to an anion type on the crystal *c* axis, that in practice is shown in lability of the structure with regard to this position.

The symmetry of XO_4^{3-} anion oscillations in a crystal lattice of apatite is determined not only by the symmetry of its local environment, but also by the nature of chemical X-O bonds inside the anion. Influence of replacement anion X (OH, F, Cl) along the *c* axis in apatite structure on the character of IR-absorption spectra is reduced to change of the amplitude of XO_4^{3-} tetrahedrons collective fluctuations that contribute to a change of the absorption bands width. The greatest influence on tetrahedral sublattice in calcium apatite renders Cl^- ion, and in strontium apatite – OH^- ion. It is also shown that the symmetry of XO_4^{3-}tetrahedrons in strontium fluoroapatite is higher compared to hydroxy- and chloroapatite.

It is shown that in the formation of the bandshape of calcium L_α-spectra in calcium apatites the significant role is played by the nuclear effects and as consequence, participation of calcium electronic *d*-states in the bond formation is levelled by their significant localization, most likely, in an internal valley of effective potential.

Correlation changes of chemical bonds in MoQ_2 (Q = S, Se, Te) with vibrational nonlinearity and overtones in Raman spectra

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The changes in the form, displacement and intensity of the main of the vibrational bands $\nu_1(E_1g)$, $\nu_2(E_2g)$ and $\nu_3(A_1g)$ in the Raman spectra of the series of dichalcogenides MoQ_2 (Q = S, Se, Te) are studied. It was established that exposure of He-Ne laser (632.8 nm), resonant with the excitonic states in MoS_2, and emission of Ar^+- laser (488 nm), incident on the edge of the electron band, lead to a strong increase of the vibrational nonlinearity (VNL). This is supported by a strong increase in intensity of the bands of 2nd order, in particular, $\nu_1+\nu_2$ and 2LA, ν_1+TA (450-460 cm^{-1}), as well as a series of overtones $n\nu_1$, $n\nu_2$ and $n\nu_3$, $n\nu_0$, where ν_0 = 40-55 cm^{-1}, (Fig. 1a). In $MoSe_2$ the intensity of high overtones $5\nu_i$-$10\nu_i$ increases significantly compared with bands of 2-3 in order in MoS_2 (Fig. 1b), which proves the strong growth of the anharmonicity and VNL. In $MoTe_2$ a series of overtones is suppressed. In MoS_2 when exposed 632.8 nm emission, besides the bands ν_2 = 382 cm^{-1} and ν_3 = 407 cm^{-1}, new bands at 395 and 419 cm^{-1} were observed, which may indicate a strengthening of chemical bonds. Structural data for MoQ_2 (Q = S, Se, Te) indicate the existence of strong internal self-compression of MoQ_2 lattice, whereby the distances between the chalcogen atoms (S, Se, Te) are significantly reduced (up to 23%) compared to the size of their ionic radii. Change of chemical bonds, in particular, strengthening of interactions between the metal atoms, is accompanied by the emergence of new electronic states in the field of vibrational overtones.

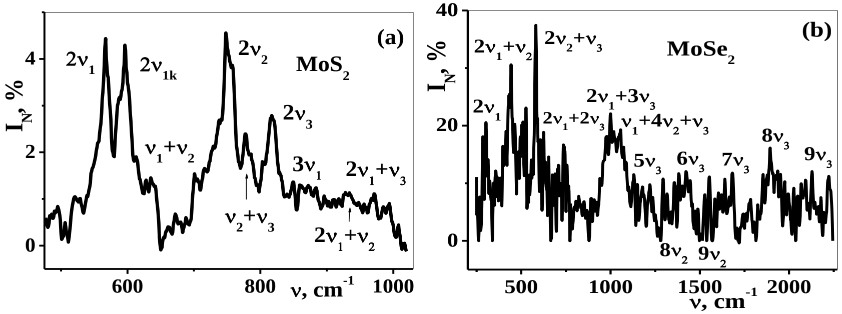

Fig. 1. A series of overtones of main vibrational bands in Raman spectra of natural MoS_2 (a) and synthetic $MoSe_2$ (b), normalized on the intensity of A_1g.

Investigation of the vibration anharmonicity in the crystal lattice of mixed composition apatites

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Contribution of anharmonic component to the broadening of the vibration bands is possible to trace on the example of the crystals, which allow making the replacement of ions without distortion of crystal structure of the lattice. Apatites belong to such crystals. The crystal structure of hydroxyl-, fluoro- and chloroapatite belongs to the spatial group $P6_3/m$, and includes tetrahedral sublattice which allows making the replacement of phosphorus by vanadium [1].

In the present work, the influence of vibration anharmonicity in the lattice of mixed composition apatites $Ca_{10}(PO_4)_{6-x}(VO_4)_x(M)_2$, where $M=OH^-$, F^-, Cl^-, x=0, 1, 3, 5, 6 on their physical and chemical characteristics is investigated using IR-spectroscopy method.

It is shown, that the change in the intensity of the IR absorption bands is proportional to the change in the relation of P and V elements in the structure of the apatite. No new bands or broadening of the bands belonging to the initial crystal structures were observed in spectra indicating that the symmetry of a lattice in samples of the mixed structure practically does not differ from that of initial forms.

It is established, that vibration anharmonicity in a lattice of apatite can change depending on the concentration of oscillators of one type in crystal structure. These changes are local, and by means of various replacements it is possible to create necessary spatial distribution of anharmonic component in the crystal that opens the prospect of controllable change of heat conductivity, factor of temperature expansion and other parameters in a crystal which depend on the vibration anharmonicity of a lattice.

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FIR spectra of the binary molibdate $KTm(MoO_4)_2$

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$KTm(MoO_4)_2$ belongs to a series of rare-earth binary molibdates. The characteristic feature of these compounds is the presence of low-temperature phase transitions caused by the cooperative Jahn-Teller effect (CJTE).

The $KTm(MoO_4)_2$ crystal has a layered crystal structure with orthorhombic symmetry (space group P_{bcn} (D^{14}_{2h})). It consists of $[Tm(MoO_4)_2]^-$ layers which are built of MoO_4 tetrahedra and TmO_8 octahedra and are separated by layers of K^+ ions.

Far-infrared (FIR) transmission spectra were measured using a commercial Fourier-transform infrared spectrometer (Bruker IFS113v), combined with a continuous-field 33-T Bitter magnet at 1.4 K in the High Field Magnet Laboratory in Nijmegen. Phonons with frequencies 16.7 cm^{-1} and 82 cm^{-1} are seen in polarization $E||a$, and 25.7 $см^{-1}$ and 109 $см^{-1}$ - in polarization $E||c$, while double peak at 86.3 and 88.5 $см^{-1}$ is seen at both polarizations. By measurements in high magnetic fields, we have confirmed the position of the first excited electronic level of Tm^{3+} ion (200 cm^{-1}) obtained in earlier heat capacity experiments [1]. Also we observed the splitting of the lowest doublet at 2.3 cm^{-1} of the Tm^{3+} ion previously studied in [2]. Low frequency phonon spectrum of the crystal $KTm(MoO_4)_2$ was calculated using one-dimension model.

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Electronic structure and magnetic properties of FeTe and $BiFeO_3$ compounds

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The iron-based compounds FeTe and $BiFeO_3$ exhibit unusual types of magnetic ordering, as well as many other peculiar electronic properties, like superconductivity (FeTe) and ferro-electricity ($BiFeO_3$). The fact that both electric and magnetic transitions in $BiFeO_3$ take place much above the room temperature makes it particularly attractive for applications. At the same time FeTe displays a unique double stripe antiferromagnetic (DS AFM) structure, with transition to ferromagnetic state at high pressures. These properties are presumably determined by specific features of their electronic structures, which are not clear up to now. Here we present results of our detailed theoretical and experimental studies of electronic structure and magnetic properties of FeTe and $BiFeO_3$ compounds.

The experimental studies have revealed unusual substantial increase of magnetic susceptibility χ under pressure for both compounds in AFM and paramagnetic phases. It is found that the anisotropy of χ is determined by specific details of the AFM transition. There are very close energies and magnetic moments for the frustrated AFM configurations. Our results indicate that the ordering of spins depends on variations of the excess iron in both compounds.

Theoretical studies of the electronic structure and the character of chemical bonds and their manifestations in magnetism have explained the ground state properties of DS AFM FeTe and multiferroic $BiFeO_3$. The dominant role of the magnetostriction mechanism is demonstrated for the coupling of magnetic and electric subsystems in $BiFeO_3$. Finally, we have calculated restructuring of Fermi surface when FeTe going from paramagnetic to antiferromagnetic phase. This explains the experimentally observed a sign change of the Hall coefficient.

The peculiarities of formation and decay of incommensurate phase under X-ray irradiation in TlInS$_2$ crystals

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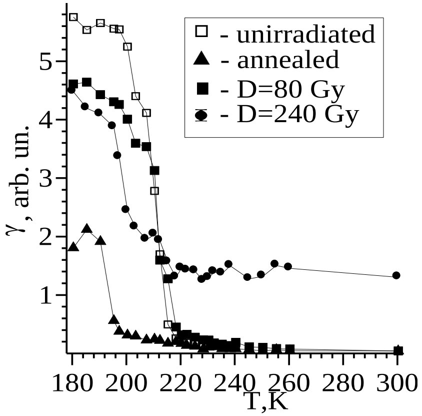
An important feature of TlInS$_2$ ferroelectrics is the existence of a sequence of phase transitions (PT) with a creation of incommensurate (ICP) and commensurate (CP) phase in temperature range T=190–240 K. Furthermore, these crystals are characterized by a large density of localized states near the Fermi level (10^{17}-10^{18}cm^{-3}), indicating about high defect concentration of different types. The defect system effects on formation and properties of ICP significantly through modulation wave pinning on defects. The state of the defect system can be changed by irradiating the crystals of electrons, γ and X-ray photons [1]. However, there is no information about structural characteristics of ICP and CP in irradiated samples in these experiments.

It was established that during the cooling in irradiated samples of TlInS$_2$ the beginning of the active formation of ICP correspond to the temperature T≈220K, and the wave vector of ICP is the same as in unirradiated samples $q(\mp 0.04, 0, \pm 0.25)$. Fig. 1 shows the ratio of the satellite $q(-0.04, 0, +0.25)$ intensity to the (405) reflection intensity $\gamma = I_{sat}/I_{(405)}$. This parameter defines the volume fraction of ICP in the sample. As can be seen, the higher the absorbed dose, the less the amount of ICP in the temperature range T=197 K-220 K, where occurs the heat generation of ICP. Also, we observed at the first time the formation of modulated structure under the irradiation dose of D=240 Gy at room temperature (circles in Fig. 1). It is important to note that an annealing the samples at T=430 K during 10 hours totally destroys this structure (triangles).



Thus, the generation of radiation defects is accompanied by appearance of the modulation wave, which might be not due to displacements of atoms, but due to periodic defect distribution in the anion sublattice of sulfur.

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Some features of incommensurate modulated structures in the $TlInS_2$ crystals

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$TlInS_2$ crystals belong to the class of thallium low-dimensional compounds $TlMX_2$ (M = Ga, In; X = Se, S, Te) and exhibit ferroelectric and semiconductor properties. Despite numerous studies the existing data on the mechanisms and temperatures of the paraelectric-incommensurate phase (IP) transition and the incommensurate-commensurate phase transition are rather contradictory [1]. So, in the present report the IP transformations in *c*-polytype of $TlInS_2$ are studied by means of the single-crystal four-circle X-ray diffraction method in the temperature range 180–300 K.

It was found that under cooling the IP satellites arise at temperature T_{i1}=238 K in plane $(h0l)^*$ as weak lines with wave vector $q(\mp\delta, 0, \pm 0.25)$ $(\delta = 0.04)$. At each temperature the index *h* of $q(4+\delta, 0, 4.75)$ satellite maximum and its integrated intensity were determined. Under cooling from 238 to 218 K the satellite intensity slightly increases, the increase being more pronounced in the temperature range of 217-213 K. The intensity sharply increases on cooling below 213 K and at 196 K the increase becomes weaker. Appreciable changes in the dependencies $I(T)$ at temperatures 213 K and 196 K are in good agreement with the known data on the phase transitions in $TlInS_2$: paraelectric-incommensurate phase at T_i=214 K and incommensurate-commensurate phase at T_c=197 K [1]. An unexpected result is the beginning of incommensurate phase formation at substantially higher temperature $T_{i1}>T_i$. We assume that the weak incommensurate phase satellites at temperatures $T_{i1}>T_i$ may be due to a distortion of the soft mode in local regions of crystal, which contains structural defects (point defects, impurity atoms and stacking faults).

It was observed the monotonically decreasing of incommensurability parameter δ at temperatures $T<204$ K. At temperature 195 K $\delta\rightarrow 0$, the commensurate phase is formed with the modulation vectors $q(0,0,\pm 0.25)$. This dependence may indicate the transition from the sinusoidal modulation to the "soliton" regime at which the distance between domain walls increases. It is typical for the incommensurate-commensurate phase transformation in incommensurate systems of type I, i.e., improper ferroelectrics with Lifshitz invariant. The model of incommensurate phase formation in c-polytypes was proposed.

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Effect of temperature on triplet luminescence of self-trapped excitons in rare-gas cryocrystals

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Radiative decay of molecular self-trapped excitons (M-STE) in rare-gas cryocrystals results in formation of molecular-like luminescence band – the so-called *M*-band. Both the triplet $^3\Sigma_u^+$ and singlet $^1\Sigma_u^+$ states of the M-STE contribute to *M*-band and decay curve of molecular luminescence yields a slow decay component and a fast one. The fast decay component is independent of temperature. The slow decay component exhibits pronounced temperature dependence because of phonon mixing of $^3\Sigma_u^+$ substates [1]. Coexistence in solid Xe and Kr of two types (intrinsic and extrinsic) of excimer-like emitting centers [2] implies different efficiency of the process of phonon mixing of $^3\Sigma_u^+$ substates depending on crystal lattice surroundings of these centers.

In the present paper we have measured decay times of M_1 and M_2 subbands of solid Xe and Kr in temperature range 10–50 K. The experiments were performed at the SUPERLUMI experimental station at HASYLAB, DESY, Hamburg. In the temperature range 10–50 K the temperature dependence of triplet lifetime may be well approximated by single exponent $\tau(T)=C\cdot\exp(D/T)$, where C and D are fitting constants. The phonon mixing of the triplet substates in M-STE independent of photon excitation energy and the temperature dependencies for subbands M_2 may be approximated by the same exponent for any excitation energy: in Xe with C_1=11 ns and D_1=45 K; in Kr with C_1=50 ns and D_1=12.8 K. But the decay of 'defect' subbands M_1 yields different temperature dependencies at different excitation energies. At excitation by photons with energies of n=1 excitons the fitting constants are – in Xe: C_2=15 ns, D_2=50 K; in Kr: C_2=58 ns, D_2=13.2 K. Whereas at excitation by photons with energies of n=2 excitons, the fitting constants are – in Xe: C_3=22 ns and D_3=51 K; in Kr: C_3=60 ns and D_3=13.3 K. The acceleration of decay of subband M_1 with increasing excitation energy is in line with analysis of relaxation of electronic excitations [3]. As excitation energy nears E_g, the trapping cross section of excitons by lattice defects, which results in subband M_1 emission, grows proportionally to $\rho^{2/3}$ (ρ is the exciton-state radius).

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Investigation of magnetic phase transition in $SmFe_3(BO_3)_4$ single crystal by Raman scattering

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The Raman scattering spectrum in the $SmFe_3(BO_3)_4$ single crystal was studied at frequencies ranged from 3.0 to 1500 cm^{-1} in a temperature range 10–300 K. Each of the $7A_1 + 19E$ phonon modes predicted by the theory group analysis was observed for the crystal of symmetry $R32$ ($z = 1$). The values of splitting between LO and TO components of polar phonons E were detected. In the region of valence vibrations of BO_3 some additional E-modes were detected which were supposed to be due to impurity centers in the crystals studied. Using different scattering geometry defined energy 8 of 12 A_2-mod. It is found that under the magnetic transition ($T_N = 33$ K) the behavior of the intensity of the line corresponding to the A_1 vibrational mode of 179.5 cm^{-1} is anomalous. No frequency changes of the phonon E-modes under the magnetic transition were observed as those in the compounds with terbium [1].

It is shown that at low temperatures the spectrum of two-magnon excitations is complex in shape and it is observed both with nondiagonal and diagonal components of the scattering tensor. This complex shape represents the peculiarities in the density of the magnetic branches. It is estimated that the magnon energy at the Brillouin zone boundary is E_m~47 cm^{-1}.

The structure of ground multiplet $^6H_{5/2}$ of a Sm^{+3} ion in paramagnetic and antiferromagnetic states and the influence magnetic phase transition on it are investigated. The obtained energies of electron transitions at 40 K (135.1 and 220.0 cm^{-1}) are in agreement with the data given in [2]. For 10 K, unlike the value 13.2 cm^{-1} reported in [2], we detected two transitions (9.9 and 16.0 cm^{-1}) the energy of which agreed with those in [3]. We observe thermoactivated transitions (125.2, 130.9 and 215.7 cm^{-1}) from these low-energy levels. The energies of electron transitions from the ground state at 10 K are 140.8 and 225.6 cm^{-1} with a strong electron-phonon interaction in the last case.

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Raman scattering in $TbAl_3(BO_3)_4$ single crystal

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Recently, rare-earth aluminum borates having good optical and nonlinear properties, which are used in laser equipment, have been investigated intensively. Furthermore, it has been found that in aluminum borate electric polarization is induced by external magnetic field.

The Raman spectra in the $TbAl_3(BO_3)_4$ single crystal were investigated in the frequency range 3–1600 см$^{-1}$ and a temperature range of 5–300 K. Analysis of the phonon spectrum and its comparison with the isomorphic compound $TbFe_3(BO_3)_4$ [1] were carried out. 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 5 K are 216.5, 276.0, 279.5, 292.0, 440.1 and 478.0 см$^{-1}$. These results agree with the data in [2] (210, 272, 275, 434 and 472 cm^{-1}) and [3] (217, 271, 275, 436 and 472 cm^{-1}) obtained by using other methods.

In the luminescence spectrum at 300 K in the energy range 14520–14660 cm^{-1} four strong lines corresponding to the transition $^5d_4 \rightarrow {}^7F_0$, were found. At 5 K the intensity of the luminescence spectrum in this region increases significantly and it becomes more complicated. Moreover, at 300 K one can observe the luminescence spectra of transitions $^5d_4 \rightarrow {}^7F_6$ and $^5d_4 \rightarrow {}^7F_5$. Its intensity is commensurate to or higher than the intensity of the Raman scattering lines. With lowering the temperature to ~160 K, the luminescence of these transitions practically disappears. Observation of luminescence from the term $^5d_4$ (20600 – 20750 cm^{-1}) on excitation by He-Ne (15803 cm^{-1}) and solid state (18797 cm^{-1}) lasers indicates strong nonlinear properties of the crystal studied.

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Raman and IR study of Jahn-Teller phase transition in $KDy(WO_4)_2$ single crystal

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Low-temperature thermal and magnetic-resonance studies show that in monoclinic $KDy(WO_4)_2$ a structural phase transition (SPT) at 6.38 K takes place [1]. This compound was studied earlier by Raman scattering method [2]. In this study we present new information on phonon and crystal-field (CF) excitations with the aim to characterize and understand the mechanism of SPT.

Raman spectra were investigated in $KDy(WO_4)_2$ single crystal in a wide frequency (3–950 cm^{-1}) and temperature (2–300 K) ranges. Infrared (IR) studies were performed in the spectral region of phonons (50–1500 cm^{-1}) at room temperature and in the wide region of CF levels of Dy^{3+} ion (3000–15000 cm^{-1}) at different temperatures (4–300 K)

All 36 Raman-active modes were found, as well as 7 CF levels of $^6H_{15/2}$ ground multuplet of Dy^{3+} ion situated at the site with C_2 symmetry. It is established that first excited electronic quasi-degenerated doublet splits at temperature higher than SPT, and, finally, has complicated structure containing four lines. This fact can indicate the presence of four nonequivalent ions of dysprosium in the low temperature phase. Moreover, three additional phonons observed at 2K are not consistent with room-temperature structure, and can indicate that primitive cell doubles at phase transition. Application of magnetic field transforms the first exited electronic doublet, which can be explained by a phase transition induced by magnetic field.

First information on IR-phonons is obtained. CF energies of Dy^{3+} ion in $KDy(WO_4)_2$ were found for 9 multiplets lying in IR region of spectrum. Dysprosium CF-levels experience noticeable shift in the temperature range 10–5 K with the most pronounced peculiarity at 6.4 K. Shift of CF energies up to 1.5-2 cm^{-1} means a change of crystal field acting on Dy^{3+} ion due to structural changes. The reason for structural changes can lie in the depopulation of the first excited CF state of Dy^{3+} ion situated at 12 cm^{-1}.

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Features of heat transfer in the «plastic» phases of isomorphic cyclic hydrocarbons

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Investigation of thermal conductivity provides important information about the dynamics of the crystal lattice. Of particular interest in this area of research are molecular crystals that have both translational and orientational disorder.

In this work we have investigated the heat transfer characteristics of the «plastic» phase of isomorphic cyclic hydrocarbons: furan (C_4H_4O) and thiophene (C_4H_4S). On the example of these isomorphous substances can be traced the influence of replacement in cycle, of the oxygen atom by a sulfur atom affects on the conductivity.

The studies are carried out in the temperature range from 80 K to melt on samples of varying densities. Purity of the samples was 99.8%. The total systematic error of measurement was dominant and did not exceed 4% for thermal conductivity and 0.2% for the volume.

Furan C_4H_4O has two phases: an orthorhombic orientationaly disordered phase I and tetragonal orientationaly ordered phase II. In phase I the temperature dependence of the isochoric thermal conductivity is significantly weaker than $\kappa \propto 1/T$, in phase II thermal conductivity increases slightly with temperature, whereas isobaric thermal conductivity decreases in both phases with increasing of temperature [1].

The isochoric thermal conductivity was measured thiophene C_4H_4S in a «plastic» phase I the three samples with different molar volumes [2]. Was found that the isochoric thermal conductivity increasing with temperature for all samples. Such behavior is typical for orientationaly disordered phases of molecular crystals and is attributed to the weakening of the translation-orientation interaction and scattering of phonons by the rotational excitations of molecules as the release of rotation in the plane of the ring.

The experimental data are discussed in the approximation of the corresponding relaxation times within a model in which the heat is transported by low-frequency phonons and by «diffusive» modes above the phonon mobility edge.

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Concentration and temperature changes of ^{127}I NQR spectrum parameters for mixed layered semiconductor crystals $(BiI_3)_{1-x}(PbI_2)_x$

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Layered semiconducting materials such as BiI_3, CdI_2, PbI_2 are known [1] to have anisotropic properties, which determines the use of those crystals as ionizing radiation detectors with a high energy resolution. In this connection, the researches of the properties (the crystal parameters) of mixed crystals $(BiI_3)_{1-x}(PbI_2)_x$ and their dependences on the content and state of PbI_2 atomic groups are challenging.

The results of the ^{127}I NQR spectrum coefficient parameters of the mixed foliated semiconductor $(BiI_3)_{1-x}(PbI_2)_x$ and their temperature in the temperature interval 77–150 K have been represented. It is shown that at the low content values of PbI_2 $x \leq 0.08$ the temperature coefficients of the quadrupole interaction constant and asymmetry parameter at the ^{127}I nuclei are not changed while NQR spectrum is changed significantly at x=0.2 and T=77 K. It is shown that at the content in the range $0 \leq x \leq 0.08$ $(BiI_3)_{1-x}(PbI_2)_x$ crystal has the properties of the impurity crystal BiI_3, which contains intralayer PbI_2 clusters, and in the range $0.9 \leq x \leq 1$ it contains intralayer clusters BiI_3. At concentrations x=0.20 and x=0.90, the $(BiI_3)_{1-x}(PbI_2)_x$ crystal undergoes a phase transition, and at the concentration of $0.2 \leq x \leq 0.9$ there is a new crystal $(BiI_3)_{(1-x)}(PbI_2)_x$ in which the groups of atoms, PbI_2 and BiI_3-intercalant are fully or partially ordered in the crystal system. Processing of the experimental results was carried out by the method of least squares according to [2].

On the basis of the fulfilled measurements, the conclusion has been made about the preservation of quasi-two-dimensional oscillating state character in the $(BiI_3)_{1-x}(PbI_2)_x$ crystal at PbI_2 content $x \leq 0.08$.

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Phonon spectra of $Pb_2P_2S_6$ quantum paraelectric with charge instability

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The ferroelectricity in $Sn_2P_2S_6$ family compounds is related to tin cation stereoactivity that appeared with local three-well potential for the spontaneous polarization fluctuations [1]. This mechanism of phase transition could be described in the frame of well-known second-order Jahn-Teller effect. For $Pb_2P_2S_6$ crystal the paraelectric phase with $P2_1/c$ symmetry (that is isostructural to $Sn_2P_2S_6$ paraelectric phase) exists at cooling until liquid helium temperature. By first-principles calculations in GGA approach of density functional theory, we found that full energy of $Pb_2P_2S_6$ paraelectric phase is only little smaller than such an energy for possible ferroelectric phase with Pc symmetry. In calculated phonon spectra of paraelectric phase, a very low energy polar optic mode with B_u symmetry at Brillouin zone center has been found. By Raman scattering, some softening of optical modes was observed in this crystal with cooling, what give evidence about growth of lattice anharmonicity. Such increase of $Pb_2P_2S_6$ crystal anharmonicity at cooling have also been found earlier as growth of Gruneisen parameter determined at elastic properties investigations by Brillouin scattering [2].

Observed behavior of $Pb_2P_2S_6$ compound could be related to the charge disproportionation phenomenon of type $P^{4+} + P^{4+} \rightarrow P^{3+} + P^{5+}$. On the matter of known valence skipping [3], the $3s^1$ electronic configuration is metastable, so it follow that the closed shell $3s^0$ and $3s^2$ electronic configurations are favorable. Such electronic localization could be considered as Kondo like behavior with participation of phonons [4]. The electronic entropy realizes at conditions of local anharmonic potential, and by this determines a growth of $Pb_2P_2S_6$ lattice polarizability at cooling across several hundreds of Kelvins. In general, the charge disproportionation could be considered as origin of ferroelectricity in whole family of $Sn_2P_2S_6$ type compounds.

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Dependence kinetic phosphorescence of ceramics ZnS-Cu from a doze of a proton irradiation

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Was studied kinetic of the light sum accumulation at an isothermal mode after an irradiation by protons of ceramics ZnS-Cu by dozes 10^{14}, 10^{15}p/sm^2 with energy 50 Mev. The excitation luminescence and the light sum accumulation were carried out by integrated study x-ray tube (Mo, 35кV, 10 mA) at temperature 85K. In work, the method accumulation of the light sum is used at increase of time of excitation. The method allows qualitatively estimating changes in system of local levels of samples.

The researches stationary luminescence have shown, that at an irradiation of initial samples the doze 10^{14}p/sm^2 observes increase of intensity roentgen luminescence (RL) and the size reserved the light sum under a curve phosphorescence (Ph) grows. The fall of intensity RL and strong reduction reserved the light sum under a curve Ph is characteristic for samples irradiated by a doze 10^{15}p/sm^2. For all three sets of samples experimental dependence’s of recession of intensity Ph after the first minute of attenuation is satisfactory approximation by hyperbolic dependence. After an irradiation of ceramics by protons has changed kinetic radiation relaxation Ph. The increase of a parameter of a degree hyperbola $\alpha = Ln(J) / Ln(t)$ is established, for the irradiated samples, where J - intensity Ph, t - the time of registration Ph, from time of excitation, in an initial sample α decreases with increase of a degree of excitation. The received dependence’s of rate of accumulation the light sum (t) during an interval of registration Ph testify to participation in attenuation of two grades of traps differing on the mechanism radiation of transitions. Moreover, the presence of radiating defects differently changes processes of the light sum accumulation on these grades of traps. For initial sites Ph τ depends on time of achievement of saturation Ph and size of intensity RL, it is supposed that this grade of a trap is a part of a uniform complex responsible for ″green″ a luminescence in ZnS-Cu. The character of change for the $\boldsymbol{\tau}$ second grade of traps explains by increase of channel recombination after a proton irradiation. The reduction increase of values τ for samples irradiated by a doze 10^{14}p/sm^2 contacts to increase of concentration interstitial of zinc (Zn_i) responsible for long low-temperature Ph. For samples irradiated by a doze 10^{15}p/sm^2 the received values t are explained by possible displacement Zn_i in regular places, that is reduction of concentration Zn_i and vacancies S.

X-ray Luminescence of ceramic ZnS-Mn

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The object of study was a fluorescent ceramics ZnS a concentration of 0.3%, 1 %, 2 % and 4% Mn in the blend. Experimental work was lying in the complex investigations of the spectrum of photo- and X-ray luminescence; of the dependencies of the stationary intensity photo- and X-ray luminescence from time and temperature of the excitation of ceramic ZnS-Mn, doze dependencies of phosphorescence ZnS-Mn. Excitation was carried out with total radiation of X-ray tube BHV-Re (20 kV, 25mA and 20kV, 5 mA) and with nitrogen laser(λ=337nm), photoluminescence excitation was carried out using a nitrogen laser (λ= 337nm). In this case, the two dominant bands were observed at λ=460 nm (blue band) and λ=590 - 600 nm. Luminescence spectrum form at photo- and X-ray excitation almost not depends from the Mn concentration. In our opinion, small difference, which we saw, caused by technological conditions of making luminescence ceramics. The main band of glow in luminescence spectrum at laser and X-ray excitation is the orange band with peak in the wavelength 600nm. In the samples with the small Mn concentrations (0.3% and 1.0%) is observing the band with the peak in the wavelength 490nm, we saw this peak on the other samples too but not so intensity. All lux-intensive characteristics (dependencies of intensity luminescence from the intensity of excitation) approximate well by the straight lines. Nevertheless, the line always pass higher than origin of coordinates is located, which can explain by presence phosphorescence during the X-ray excitation. The phosphorescence curves for the same dose of X-ray excitation, but with the different intensity and time of the excitation, do not match. Besides the difference with them is increase with the increase of the radiation time. Phosphorescence intensity depends not only from dose, but from time of radiation too. The curves of the phosphorescence with the smallest dose of radiation well described by hyperbolic dependence, unlike curves with the time of radiation more than 120 seconds. The phosphorescence at 85K occurs through delocalization carriers from trap, which is a manifest in form of first peak thermally stimulated luminescence. The index of the hyperbola quenching phosphorescence for the curves after the X-ray quantum’s radiation for all dose emission less than one (α<1), for the curves after laser emission more than one (α>1). The dose phosphorescence dependences at the X-ray excitation could not explain in the classical kinetic theory of the photoluminescence and in kinetic theory of x-ray luminescence. The study of the emission bands of increased interest due to the practical use of ZnS-Mn as an effective semiconductor element MDM structures that are widely used in light indicator displays.

The role of periodicity and effects of disorder in the vibrational spectra of synthetic opals

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Synthetic opal (SO) is one of the most famous representatives of photonic crystals [1]. Optical properties of silica opals, are dependent strongly on the substructure and packing type of their globules, concentration defects.

In this work we have studied infrared (IR) spectra of synthetic opal with different type of ordering and after rough treatment. IR spectroscopy gives info about structure of globules, ordering and impurity of SO. Early we have studied the IR spectra of different form of silica (fused silica and ⟨-quartz) in comparison with IR spectra of SO globules [2].

We found a narrowing of the phonon band of ordering PC in comparison with disordering SO. The half-width of the stretching vibration band (1100-1300cm^{-1}) for ordering i SO s 88cm^{-1} and less than disordering SO, namely, 95cm^{1}. For disordered structure (in literature named photon glass) half-width consist – 123 cm^{-1}. That is why, this band could be used as marker of perfectness of SO structure. Data of IR spectroscopy provide information on the presence of impurities of extremely small amount.

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The thermal conductivity of a fractal nanostructure in simple molecular solids

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The thermal conductivity of molecular solid and exotic phases of solid alcohols (ethanol, 1-butanol and cyclohexanol) and 2-adamantane has been measured.[1-3] It is shown that the behavior of the temperature dependence of the thermal conductivity of metastable solids differs drastically from that in the amorphous state and the ordered phase. The effect of annealing and thermal conductivity relaxation has been detected in the orientationally ordered phase. It has found that thermal conductivity of metastable molecular solids obtained by crystallizing a deeply supercooled state exhibits a nontypical low-temperature dependence. This dependence is characteristic of fractal nanostructures.

5

Liquid Crystals

Electro-optical effect in the nematic cell with tunable boundary conditions

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The plane nematic cell with strong planar anchoring on the lower cell surface and finite anchoring on the upper surface was considered. The Freedericksz transition in static electric field perpendicular to the cell boundary planes was investigated theoretically, assuming that the easy axis of director orientation on the upper surface interacts with external electric field having Rapini-like potential.

It was shown that the threshold voltage is more than two times smaller in comparison with the case of Freedericksz transition with the strong anchoring on both boundaries. It was also shown that for some parameter values in the threshold point the director can abruptly change orientation from homogenous to inhomogenous state.

The investigation of light transmittance through the cell was carried out in case of normal incidence of linear polarized monochromatic light beam. The light intensity at the outlet of the cell as a function of applied voltage was obtained for different values of interaction strength between easy axis and external field.

Mixtures of 5CB and azoxy nematics as hosts for dispersion of carbon nanotubes

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One of the ways for improving application prospects of nanomaterials based on liquid crystal (LC) – carbon nanotubes (CNT) dispersions is to use LC hosts with peculiar properties that eventually could be enhanced by the presence of CNTs. In this work, we used mixtures of 5CB and azoxy nematic ZhK-440. In such mixtures, formation of charge transfer complexes between azoxy and cyanobiphenyl molecules occurs, which leads to formation of induced smectics in the concentration interval around 50%. From the other hand, these nematics have opposite signs of dielectric anisotropy $\Delta\varepsilon$, and the expected compensation point should be about ~10-12%.

In our experiments, several characteristics (electric conductivity, optical transmission, perpendicular component of ε) measured in planar geometry as functions of 5CB concentration showed well-defined singularities close to the $\Delta\varepsilon$ compensation point (sharp decreases in conductivity and transmission, and a certain increase in the measured ε). At higher concentrations of 5CB, Freedericks-type transition was clearly observed under application of dc electric field, resulting in homeotropic orientation of the nematic molecules; the accompanying changes in conductivity and ε were substantially increased upon introduction of CNTs. As a next step, helically twisted (cholesteric) structure was achieved by adding chiral components (cholesterol esters) to the nematic mixture. In this case, photoinduced effects of texture transformations could be observed under electric field stabilizing the homeotropic orientation. Possible implications and applications of such a “photoelectrooptic” effect are discussed.

Dependence of lasing characteristics of dyed CLC on mutual orientation of directors at orienting substrates

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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 CLC lasing, when 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 its radiation was presented by three longitudinal modes with small changes under practically available optical pumping. Spatial radiation pattern corresponds to the transverse modes of a ring structure Laquerre - Gaussian nature.

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 spiral structure type "phase jump" [2], which can occur in such a viscous medium and affects the lasing spectra.

Also the lasing characteristics of CLC with macroscopic isotropic layer in cavity potentially considered as a defect of the photonic crystal have been examined.

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Dispersions of carbon nanotubes in cholesteric liquid crystals with azoxy nematics as photoactive components

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Optical transmission and selective reflection data are reported for dispersions of single-walled carbon nanotubes (SWCNT) in cholesteric liquid crystals comprising a mixture of cholesterol esters and azoxy nematic ZhK-440. As distinct from similar dispersions in 5CB or ZhK-440, where optical density could be described basing on the Bouguer-Lambert-Beer law [1], in this case the optical density D was essentially non-linear with SWCNT concentration c. The initial rise of $D(c)$ was followed, after reaching a certain threshold concentration, by a sharp fall, with subsequent further increase in D. The observed behaviour was ascribed to formation of "stacked" aggregates of nanotubes. A molecular model is proposed, illustrating the difference between NT aggregation in nematics (where fractal aggregates are formed at higher CNT concentration) and cholesterics (where formation of fractal aggregates is suppressed).

The location of this minimum on $D(c)$ plots, as well as selective reflection maximum (helical pitch) in these systems are sensitive to partially reversible UV-induced *trans-cis-trans* isomerisation effects of the azoxy molecules. The total (equilibrium) magnitude of the UV-controlled helical pitch variation was only slightly affected by introduction of carbon nanotubes. However, CNTs substantially modified kinetic characteristics of this process – the initial rate of the direct (*trans-cis*) transformation was noticeably increased, and hysteresis effects were noted for the inverse (*cis-trans*) stage. Application prospects of such materials in optoelectronic devices are considered.

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Director distribution and defects location in a nematic cell with corrugated surface

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The nematic cell the upper surface of which is plane and the lower one consists of a set of long parallel grooves with the sine-like profile was considered. The anchoring strength between the nematic director and surfaces was assumed to be strong: planar on the upper surface (an easy axis is perpendicular to grooves' direction) and homeotropic on the lower surface. Assuming plane director field deformations, an exact expression for director distribution in the cell was obtained in the one elastic constant approximation. Due to the stiffness of the boundary conditions topological defects – disclination lines have to appear above the crests and troughs of the grooves. Minimizing the free energy of the system numerically the equilibrium location of the defects was found. It was shown that the distance between the defects and the lower surface decreases as the depth of the grooves grows. For sufficiently thick cells (in comparison with grooves spatial period) the defects location doesn't depend on cell thickness i.e. the defects “stick” to the corrugated surface.

Time Domain Spectroscopy of chosen Nematic Liquid Crystal Compunds in 03. - 3.0 THz

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Liquid crystal materials have interesting properties in THz wave range [1-3]. The structure and rotational and vibrational oscillations of liquid crystal molecules have influence on physical properties of the material in this frequency range. Some liquid crystal materials obtained in Institute of Chemistry Military University of Technology with high polarization coefficients more that 2000 nC/cm2 were prepared. Special transducers made of quartz glass and silicon for measurements process were prepared.

Liquid crystal materials with relatively high dielectric anisotropy parameters ($\Delta\varepsilon$ form 0 to more than 30) and optical refractive index (Δn from 0 to about 0.6) were investigated looking for application properties. Time Domain Spectroscopy measurements were used [2]. Dielectric properties and refractive index were determined. Significant differences in their dielectric losses and tunability have been obtained.

Dependences between molecular structure and physical parameters were find and discuss [1].

Acceptable parameters looking from application point of view were received. This kind of liquid crystal samples can have application in tunable terahertz devices [3].

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Control of plasmons in graphene microarray by using liquid crystal

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Although the noble metals dominate the literature on plasmonics, graphene plasmons quickly turn into a viable tool for manipulation of light from NIR to THz frequencies [1]. Attractive properties of graphene are: smaller optical losses in THz spectral region as compared with noble metals, ultrafast carrier relaxation time, electrical tunability, fast plasmon modulation, negative and positive values of conductivity in different spectral ranges depending on chemical potential.

Growing attention is paid to tunable plasmon excitations and light–plasmon coupling at THz frequencies in graphene micro-ribbon arrays. In particular, the configurations were considered, wherein graphene surface plasmons induced absorption is enhanced [2].

In present work, we consider the system liquid crystal (LC) - periodic array of graphene micro ribbons – dielectric. The aim of the work is to study the impact of reorientation of the LC director on adsorption, reflection and transmission spectra in the terahertz frequency range at normal incidence of light. The novelty is that for studying resonance diffraction in the periodic array of graphene microribbons under excitation of graphene surface plasmons we for the first time include the liquid crystal.

We show that increasing the director angle of nematic LC leads to decreasing of reflectivity, increasing of absorption and transmission of the incident light, which normally falls on the system in the THz frequency range. Decrease in the dielectric constant of the substrate leads to a blue shift of the spectrum.

Our analysis can be used to enhance characteristics of graphene-based applications, for example, ultra-thin voltage and LC-controllable THz absorbers.

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Electric external fields act on the liquid crystalline layers, modifying their degree of order

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Liquid crystalline layers are usually obtained by collective dipolar interactions between the mesogen molecules. Both the orientation order (for nematics, lyotropics or cholesterics) and also positional order (in the case of smectics) characterize the liquid crystalline samples. Liquid crystals characterized by orientation order have the preferential direction parallel to the long axis of the mesogen molecules and can act as uniax anisotropic layers.

Liquid crystalline layers can change the polarization state of light. The changes in the polarization state can be evidenced using a device consisting from two crossed polarizers having between them a cell with liquid crystalline layer. Some visible radiations can keep their polarization state (the electric field intensity is parallel to the transmission direction of the polarizer) and the other for which the electric field intensity become perpendicular on the transmission direction of the analyzer. The first components do not pass through the second polarizer (analyzer) and the second pass in the maximum of transmission. The signals recorded by a spectrophotometer give channeled spectra from which the linear birefringence and its dispersion can be determined.

The electrostatic external electric field has been applied between the interior walls of the cell containing the liquid crystal, perpendicular on the cell and parallel to the light propagation direction. The long axes of the mesogen molecules were oriented parallel to the cell walls. The electrostatic field increased the orientation degree of the mesogen molecules by dipolar interactions

This method was used in the case of transparent liquid crystalline layers and it is applied to compute the compensatory wedges or layers and also to appreciate the effect of the electrostatic field on the liquid crystalline layers linear birefringence.

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Specific properties of liquid crystals with hydrogen bonds in confined volume

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For recent decades, the unique physical properties of the liquid crystals in confined volume are the subject of great interests since they are very different from those in their balk state. This can be used to find new nanocomposite materials with desired properties for the needs of microelectronics, catalysis, optical devices and other applications tasks. Understanding the molecular mechanisms of interaction between the liquid crystal molecules with active centers of the mesoporous matrix will make it possible to manage and control the properties of the nanocomposites and develop their commercial applications.

Since the stability of nanocomposite materials depends significantly on the bonding strength between the organic and inorganic components, the aim of this study was to investigate a new class of LCs - hydrogen-bonded LCs - confined to solid mesoporous matrices based on silicon oxide (molecular sieves AlMCM-41, MCM-48, SBA-15, KIT-6 with different geometry and pore sizes). The results of FTIR spectroscopy and differential scanning calorimetry investigation of *4*-hexylbenzoic C_6H_{13}-C_6H_4-COOH (4-HBA) and *4*-butylcyclohexanecarboxylic C_4H_9-C_6H_{10}-COOH (4-BCA) acids incorporated into AlMCM-41 molecular sieves are discussed. It was found that no crystallization or mesophase formation is observed for neither compound confined in AlMCM-41. It was also shown that Lewis acid sites on the AlMCM-41 pore surface are able to deprotonate the carboxylic acid group of some part of the LC molecules to form the carboxylate ions $R\text{-}COO^-$ which then are bonded to AlMCM-41 pore surface via coordination bond $R\text{-}COO^- {+} Al^+$. The other part of the LC molecules inside the pores stays in undissociated bulk-like state being assembled in open dimers or chain associates. The mechanisms of the LCs anchoring and orientation on the pore surface of other matrices are discussed.

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Transport properties of ionic thermotropic liquid crystals

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Ionic liquid crystals (ILC) of metal alcanoates form insufficiently explored group of liquid crystals, which have a number of advantages comparing to traditional molecular liquid crystals. Most uni- and divalent metal alkanoates form ionic liquid crystals of smectic A type while melting [1]. These compounds are perspective for the developing systems of information recording due to their own ionic conductivity, high solvent capability, good thermal stability and ability to form mesomorphic smectic glasses [2]. The particular feature of these compounds is the possibility of separate existence of cationic and anionic parts of molecules in mesomorphic phase (in contrast to molecular liquid crystals in which metal is strongly screened by atoms of ligands). This causes an occurrence of new properties in such phases.

In this work we have for an object studying of transport properties of ionic thermotropic liquid crystals (ITLC) of cobalt decanoate, lead decanoate and their binary admixture. It was obtained that both ITLC and binary mixture are weak electrolytes (in the temperature region of mesophase existence). The above mentioned compounds are characterized by the presence of the great anisotropy of bulk a conductance. It is shown that metal cations are dominating charge carriers. Also the charge mobility and concentration in polydomain samples were determined.

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Blue phases of pure cholesteric liquid crystals with a wide range of near-room temperature

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The phase transitions of pure cholesteric liquid crystals, based on right- or left-handed chiral dopants (non-mesogen enantiomers R-811 and S-811) with various concentrations dissolving in the nematic liquid crystal mixture CHCA (ZhK-805 consisting with hexancarboxylic acid dimers) were prepared and experimentally studied.

For the first time, blue phases of cholesterics were found at the concentration range of chiral dopants 32 ÷ 36 wt.%. Experimentally it was observed that during the cooling process the blue phase of cholesterics, based on 33 wt.% of chiral dopants, is stable over a wide temperature range about ~ 15^{o}C including human body and near-room temperatures.

Thermal phase transitions, spectral characteristics and electro-optical features of blue phases were examined. Planar and homeotropic alignment layers were used to study the influence of various boundary conditions on platelet textures of blue phases.

Electro-optical effect in nematic liquid crystal in homeotropic-planar Freedericksz transition

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Nowadays scientists pay much attention to liquid crystals because of their various possibilities of practical use in different fields of technology. Grand interest to physics of processes in the nematic liquid crystal (NLC) cells in external fields, and in particular to threshold effects (Freedericksz transition), is primarily associated with wide use of these cells in a variety of electro-optical devices for displaying information [1, 2].

We studied the electro-optical effect on orientation of nematic liquid crystal cell with controlled boundary conditions. We consider homeotropic NLC cell that is placed in homogeneous external electric field which is oriented towards the cell surface. It’s assumed that molecules of polymer coating of the cell surface have their own dipole moments, so their interaction with external electric field results in change the direction of easy axis. Obviously, this fact affects the value of light transmission in the NLC cell. The novelty is that such interaction of easy axis of director with external field was considered for the first time.

The threshold instability of director orientation and its dependence on the value of interaction coefficient of easy axis with external electric field was found. The calculation of the director field under the threshold and transmission coefficient of light through the cell was made.

For some values of parameters of NLC cell, interaction of the easy axis with external electric field can leads to jump-like change of deflection angle of director with increasing the applied voltage.

The coefficient of light transmission of the cell in the case of normal incidence was calculated. The influence of finiteness of coupling energy of nematic liquid crystal with cell surface was investigated. We showed that the interaction of easy axis with the electric field in two or more times decrease the threshold value compared with the case of absence of such interaction.

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Light-induced liquid crystal director freezing on inorganic chalcogenide nano-surface

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We report the first observation of light-induced angular patterns formation in a planar liquid crystal (LC) cell with chalcogenide film as orientation layer. The angular patterns appear under the irradiation of the chalcogenide surface by gaussian laser beam through the LC layer. The experimental results are explained in terms of the transfer of heat from the chalcogenide film to the LC after the light absorption in the chalcogenide layer. Light-induced heating causes a change of the birefringence of the LC and, as a result, spatially modulated polarization state in the plane of the chalcogenide layer. Since the chalcogenide film is a photoaligning material, the spatial modulation of the light polarization leads to a formation of the spatially modulated easy orientation axis and the ring structure of the director in the cell.

The effect of static electric field on hysteresis of light-induced Freedericksz transition in nematic liquid crystal cell

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The impact of external static electric field on hysteresis of light-induced Freedericksz transition in nematic liquid crystal cell in the field of light beam with restricted width is considered. External electric field is parallel to incident light polarization. Cases with parallel and perpendicular orientation of electric field to cell surfaces are shown. Threshold values of Freedericksz transition are computed for increasing and decreasing electric field tension and width of light beam. The range of light beam width and electric field tension when Freedericksz transition has a hysteresis is defined. Experimentally measured values of the width of hysteresis loop of light-induced Freedericksz transition are compared with computed results in dependence on light beam width for several kinds of nematic liquid crystal. It is shown that hysteresis loop and range of appropriated values of light beam width extend with increasing static electric field tension when field is perpendicular to cell surfaces and in contrary narrow when electric field is parallel to cell surfaces.

Phototuning of frequency of CLC-laser and ways of its optimization

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Lasers based on dye-doped cholesteric liquid crystals (CLC), were first discovered in [1]. With main lasing characteristics achieved at the present time, such lasers can be really used in displays of high brightness. Pressing problem in such lasers is the absence of rapid method of lasing frequency tuning. Temperature change of the helix pitch, which was used up to now, appeared to be very inertial.

Here we report on the results of our research on phototuning of lasing frequency in induced CLC by changing concentration of azo- and azoxy-groups of photoisomers with its selective irradiation. With using nematics containing azoxy groups, such as ZhK-440 and ZhK-654, in which twisting impurities are cholesterol esters (without photoisomers), the conditions to minimize the lasing threshold are investigated. The lasing frequency tuning range is achieved of up to 43 nm forward and 35 nm in reverse. The ten minutes time of the lasing frequency tuning in these LCL is registered due to the proximity of the absorption bands of both stereoisomer’s.

A significant decrease in the phototuning time is obtained by using highly sensitive Li-7 twisting impurity, which absorbs light at the frequency of the excitation laser.

For the first time, coherent light generation is detected in Li-7- induced CLC. A record-short time for the lasing wavelength tuning (by 21 nm in 148 ms) is achieved under the CLC irradiation with a diode laser at 532 nm wavelength. Thus, a reduce in the phototuning time by almost 3 orders of magnitude compared to known CLC materials is obtained [2].

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The interaction of electromagnetic waves in nematic liquid crystal waveguides

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The interaction of coupled TE-modes on the diffraction grating of director in a plane waveguide with nematic liquid crystal layer is theoretically investigated. Diffraction grating in the nematic layer is created by external electric field due to the periodicity of anchoring energy of director with waveguide surfaces. Metal and dielectric waveguide cases are considered. The dependence of signal mode intensity at the output of nematic layer on the amplitude and period of anchoring energy, sizes of nematic layer and electric field tension is computed. Parallel and antiparallel modes cases are represented. Analytical expressions for maximal signal mode intensity are obtained. In the case of interaction of coupled antiparallel modes in metal as well as in dielectric waveguides the main maximum of signal mode intensity increases with the number s of anchoring energy periods on the length of nematic layer and reaches the highest value if s is about several tens for metal waveguide and is about thousand for dielectric one. In the case of parallel modes, the main maximum of signal mode intensity oscillates with enhancing s. The main maximum of signal mode intensity monotonously increases with electric field tension in all cases.

Infrared study of molecular associates and isomers of cholesteryl formiate

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Cholesteryl formiat (ChF) is the first member of cholesteryl n-alkanoates homologous series. ChF has a monotropic cholesteric liquid crystalline phase which appears under cooling of the isotropic phase [1]. IR spectra have shown [2, 3] that in ChF there are intermolecular hydrogen bonds. The purpose of the present work is study molecular associates and isomers of ChF.

ChF in solid crystal, cholesteric liquid crystal, and isotropic liquid phases as well as in solution in the CCl_4 was investigated by IR spectroscopic method. Infrared absorption spectra in the 4000-400 cm^{-1} range were measured with UR-20 spectrophotometer.

IR spectra show that in solid crystalline phase at 295 K all molecules of ChF are associated in dimers by means of intermolecular hydrogen bonds. At higher temperatures in solid crystalline, liquid crystal and isotropic liquid phases, ChF molecules are in the form of dimers, *trans*- and *cis*-isomeric monomers. Their relative concentrations in different phases are determined by IR spectra. Conformational equilibrium dimer–*trans*-isomeric monomer–*cis*-isomeric monomer is displaced to the right with temperature increasing.

From the temperature dependence of intensity of IR spectra, the difference in the energy of different isomers was estimated and appeared to make up 0.6 kJ/mol. At high temperatures, slightly different in energy ChF isomers are in dynamic equilibrium. In solid crystalline state at 295 K, *trans*-isomers are stabilized by intermolecular hydrogen bonds.

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6

Methods & Applications

Random lasing and its application in Raman spectroscopy

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Random lasing (RL) is the emission with laser-like behavior arising in a dyed multiply scattering medium (MSM) under high pumping. Multiple scattering of the emitted light substitutes reflection of it off a cavity mirror inconventional laser. Due to this feature the RL radiation is undirectional and has continuous spectrum. These pecularities may be succesfully applied in laser spectroscopy to study Raman spectra of laser dyes. This problem is important because dye luminescence hampers utilization of conventional Raman method. Important advantage of the RL is that intensive radiation of continuous spectrum can arise in the same studied medium. This radiation and incident monochromatic pump form bichromatic exitation of all molecule vibrations whose Stokes frequencies appear in RL spectrum. It produces conditions which are similar to CARS (coherent antistokes Raman scattering) technique but in Stokes region and using single sourse of pump. It causes stimulated Raman scattering (SRS) of dye at mentioned frequencies what may be used for obtaining of vibrational spectrum.

For this usage we investigated peculiarities of RL and SRS excitation by it of several laser dyes in different MSM: concentrated suspensions of dielectric microparticles in polymer, vesicular polymeric films and “photon boxes” (dyed polymer covered by highly reflective dielectric microparticles). It was found that the best conditions for RL emergence and SRS are realized in vesicular films where areas of RL, SRS and dye exciting practically coincide. Important parameters influencing SRS are temperature, concentration of dye and vesicles. This influence is realized through reabsorption and reemission of emitted light and change of effective gain. Required condition for RL assistance of SRS initiation is intersection occurence of RL spectrum and of area of Stokes lines which may be found using vibrational frequencies of IR absorption spectrum.Observed SRS is resonant: pump radiation frequency must coincide with dye absorption band.

Nonlinear physical processes in critical fluid is the basis of their practical use in the novel technologies

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A number of the nonlinear physical phenomena occurring in the inhomogeneous critical fluid under the influence of the internal non-uniform electromagnetic field $|\Delta U(h)|>>|h|$ [1] induced by external field of gravity of the Earth ($h=\rho_c g\Delta z/P_c$) have been studied work. The new method of measurements of a high-altitude gradient of the internal field dU/dh has been proposed by micro-float manometer [3]. It has been shown that under the influence of this internal non-uniform field in the critical fluid it is the focusing the light beam propagation through spatially inhomogeneous system, the change in the critical temperature of substance T_c and in the critical index of coexistence curve β.

Using the data of intensity of scattered light [1,3] the correlation length (R_c), number of fluctuations of the order parameter per mole of substance ($N_f \sim R_c^{-3}$), substance density within fluctuation the order parameter ($\rho_f \geq 3\rho_c$), intramolecular pressure in fluctuation volume ($P_f \approx 10^2 P_c$), great thermodynamic potential ($\Omega = -P_f V_c$) and its fluctuation part ($F_f = N_f k_B T$) connected with the work of formation of the order parameter fluctuation ($A \approx F_f$) have been calculated. It has been shown that during the decay of fluctuations of the order parameter the molecules of substance scatter with rates of spread $\upsilon \approx 10^6 \div 10^7$ cm/s [3], comparable with the escape velocity. The conclusion is made that such high speed of molecules of substance is the basis of the successful use of unique properties of the critical fluid in novel industrial technologies [4].

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β-ketoenole dyes for detection of proteins amyloid aggregates

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The protein amyloid aggregates are associated with the pathogenesis of the range of human diseases and search of analytical tools for their detection and investigation is an actual assignment.

Here we report a study of the series of ten β-ketoenole dyes as fluorescent probes for detection of amyloid aggregates using model fibrillogenic proteins insulin and lysozyme. For this, the spectral-luminescent properties of β-ketoenole dyes in the presence native insulin and lysozyme and proteins aggregates into the amyloid fibrils were explored and compared.

The dyes contain variety of functional amino-substituents of different chemical nature and spatial geometry all of them are weakly fluorescent when free. These dyes give fluorescent response on the presence of protein amyloid aggregates and increase their emission intensity up to 25 times, while they are slightly sensitive to the presence of native proteins. The absorption maxima for these dyes are located in the range 410-430 nm and emission maxima in the range 530-550 nm. The β-ketoenole compounds possess the large values of Stokes shifts up to 75-147 nm, that is an advantage of these dyes as potential fluorescent probes.

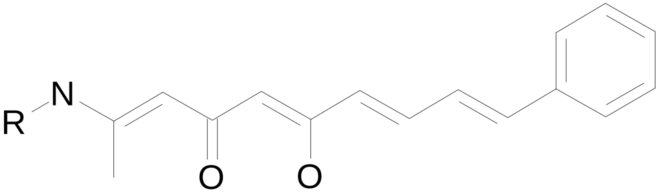

Fig.1 The chemical structure of β-ketoenole dye (R – different substituents).

The fluorescent sensitivity of these compounds to fibrillar proteins depends strongly of the nature of their functional substitutens, the most pronounced response is given by dyes that carry “short” alkyl or hydroxyalkyl and aminoalkyl tail groups.

Thus we consider that β-ketoenole dyes are prospective as fluorescent probes for the detection of the β-pleated protein aggregates.

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Frequency-shifted feedback diode lasers for molecular spectroscopy

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Laser frequency combs have revolutionized precise measurements of frequency and time. The regular pulse train of a broadband laser can give rise to a regular comb spectrum of millions of laser modes with spacing precisely equal to the pulse repetition frequency. Frequency combs are now becoming enabling tools for an increasing number of applications, from the calibration of astronomical spectrographs to molecular spectroscopy. The broad spectral bandwidth and the high-resolution structure of a frequency comb indeed make it an attractive tool for broadband direct absorption molecular spectroscopy.

In this paper we represent frequency-shifted feedback (FSF) diode laser with seeded laser what one can use in direct absorption frequency comb spectroscopy. The spectrum of FSF laser with seeded laser is the comb or, by another words, is the set of discrete frequency components where lowest frequency component coincides with frequency of seeded laser and the interval among neighbour components is determined by AOM frequency.

Centre wavelength of the laser generation is 780 nm. Output power of laser is 20 mW. Main element of FSF laser is AR-coated laser diode Toptica LD-0780-0050-AR1 with reflection coefficient 10^{-4} of output surface. Frequency shift is produced by acousto-optic modulator Neos 23080-1 (acoustic frequency 80 MHz). AOM is aligned for providing of up-shifting of radiation frequency. For the generation of required bandwidth diffraction grating Thorlabs GR25-1208 is placed inside the cavity in Littrow configuration. The bandwidth of FSF laser spectrum is 9 GHz. The broadband tuning is ensured by rotation of grating in horizontal plane, fine tuning – by variation of diode laser injection current.

Seeded laser is tuneable single frequency laser. This laser is constructed on Littmann-Metcalf cavity configuration and consists of diode laser Thorlabs L780P010, grazing-incidence grating Thorlabs GR25-1208 and high reflection mirror. The tuning of wavelengths of seeded laser to wavelength of FSF laser is ensured by rotation of mirror in horizontal plane, fine tuning – by piezoelectric shifting of mirror and by corresponding variation of diode laser injection current.

Positron annihilation lifetime spectroscopy in application to nanoporous structural characterization of MgO-Al_2O_3ceramics

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The nanostructured spinel MgO-Al_2O_3 ceramics are widely used as one of the most perspective materials for humidity sensors. It is established, that structural features (free volume and evolution of nanopore structure) and humidity sensitivity of these ceramics depend on their sintering route. With this in mind, we studied the correlation between sintering temperature of ceramics and evolution of their free-volume (sizes of nanopores) with using of positron annihilation lifetime spectroscopy PAL (ORTEC spectrometer with ^{22}Na source).

The studied ceramics were sintered in a special regime with maximal temperatures 1100, 1200, 1300 and 1400 °C. The initial powders of Al_2O_3 and MgO were used as starting components within conventional ceramics technology route. Before studying the experimental samples were exposed to the water vapor in desiccators at relative humidity of 100 %. PAL measurements were performed after drying of ceramic samples in vacuum at 120 °C for 4 h. The obtained PAL spectra were mathematically treated with LT computer program using four-component fitting procedure. The size of nanopores for $MgAl_2O_4$ ceramics in spherical, cylinder approximation can be calculated using well known model Tao-Eldrupa. It was established that free volume radius calculated is near 3.0 Å in ceramics sintered at 1100°C and increase to 3.3 Å for ceramics sintered at 1400°C.

IR-spectroscopy studies of Mn-Bi-Cu-Ce-O catalyst for low-temperature oxidation of ammonia to nitrous oxide

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Selective catalytic oxidation of ammonia (NH_3) with air at low temperatures is an efficient method to produce N_2O as oxidizing agent for organic synthesis. This process has two important parameters: the selectivity and the application temperature. To rationally develop a process for NH_3 oxidation to N_2O over catalysts, the reaction mechanism must be clarified. While several studies have examined the low temperature oxidation process, the mechanism of NH_3 oxidation and N_2O formation is still uncertain. Generally, an imide (NH) mechanism is used, in which the first step yields NH, and then the NH reacts with atomic oxygen (O) to form nitroxyl (HNO) and further conversion to N_2 or nitrous oxide (N_2O), or NH could even react with molecular O_2 to produce nitric oxide (NO) [1].

In the present paper the influence of catalyst composition and some operating variables were evaluated by IR-spectroscopy in terms of N_2O formation, using Mn-Bi-Cu-Ce-O catalyst. The IR spectra of ammonia adsorbed on the catalysts show the bands at 1594 and 1165 cm^{-1}, which attributed to σ_{as} and σ_s model of NH_3 coordinated to Lewis acid sites. Another two bands at 1674 and 1445 cm^{-1} are attributed to σ_s NH_4^+ and σ_{as} NH_4^+ resulting from ammonia coordinated to Brønsted acid sites [2]. It is indicated by the increase in intensity of band at 1165 cm^{-1} that more Lewis acid sites are generated on Mn-Bi-Cu-Ce-O by introduction of Ce^{x+} which can also serve as Lewis acid sites. Comparison of IR spectra from catalyst treated with 1000 ppm NO, 1000 ppm NO_2, and 1000 ppm NO + 2% O_2 shows the five bands at 1610, 1550, 1466, 1291, and 1030 cm^{-1}. The bands at 1550, 1291, and 1030 cm^{-1} can be assigned to bidentate nitrate; the band at 1466 cm^{-1} can be attributed to the monodentate nitrite [3]. The mechanism proposed for N_2O generation at low temperature is based on the formation of surface Ce-ON species which may be produced by the partial oxidation of dissociatively adsorbed ammonia species with NO + O_2 (eventually NO_2) [4]. When these active sites are in close proximity they can interact to form an N_2O molecule.

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Nonlinear optical characterization of laser phosphate glasses by the self-action of picosecond laser radiation

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Glassy materials with a high luminescence quantum yield, suppressed nonlinear-optical (NLO) response, improved thermo-optical characteristics and a low crystallization propensity are of special interest for the production of large-sized workpiece by conventional methods. Such glassy optical materials may be prepared by substitution of Ba for Sr that can be done in the whole range of the composition of exchangeable Ba/Sr-based multicomponent laser phosphate glasses containing Nd^{3+}. An important aspect of improving laser phosphate glass characteristics is to reduce the nonlinear refractive index coefficient n_2. It can be achieved by composition modification of the glass. Low efficiency of the nonlinear refractive response can reduce the probability of the light-wave front distortion, which is especially important at high irradiation densities. Improving of such characteristics, as the extinction coefficient at the wavelength 1053 nm, can be achieved by using of a high purity raw materials and advanced methods of the glasses processing. Necessary technological level of production was achieved by using specially elaborated methods of the separation of admixtures and of the purification of the initial reagents. The latter are composed a butch mixture used to obtain the laser glasses of a high purity.

The NLO response of the samples was studied within the spatial profile analysis technique under the irradiation of picosecond laser pulses at 1064 nm. This approach demonstrated earlier a high sensitivity to the substitution of the Lu atoms by Gd in the oxyorthosilicates single crystals [1]. It was shown the correlation of the refractive NLO response efficiency with the ratio of Sr/Ba in the laser phosphate glasses. The magnitude of $n_2 \sim \mathrm{Re}(\chi^{(3)})$ increases as the Sr content decreases. On the basis of the obtained results we suggest a high potential of the application of the pulsed laser radiation self-action effects for the characterization of the laser phosphate glasses.

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The influence of artificial lighting on the growth characteristics of biological objects

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Light is one of the important factors of growth and morphogenesis of many species of fungi. As temperature and humidity, light belongs to the environmental factors that affect their vital functions. Thus, the results of numerous studies suggest the possibility of implementing highly efficient biotechnology based on the use of artificial lighting for plants with high biological activity, increased cellular and extracellular content of biological products. In [1] it has been investigated the influence of irradiation by light emission diodes (LEDs) on the mushroom’s growth.

Given the principles of creation of artificial lighting systems for use in plant and on the basis of known data about photosensitivity of mushrooms developed setup for formation of luminous flux with desired parameters using high intensity light emission diodes. LED matrix formed from twenty-one LEDs based AlGaInN type YSH-FRGBB-IA manufactured by China Young Sun Led Technology Ltd. Each one had three light-emitting microchips with emission wavelengths 463 nm (blue), 522 nm (green) and 625 nm (red). Maximum electric power of each microchip was 1 W. One of the aims of our research was to find the ways for intensification of the cultivation process of *Pleurotus ostreatus* due to increased physiological activity of sowing mycelium. Work was conducted with strain 431, which is used in industrial mushrooming in Ukraine.

Study of nature of substrate growth inoculated by unirradiated and irradiated with different doses of light mycelium *Pleurotus ostreatus*, made it possible to establish that the irradiation of mycelium leads to full substrate growth in a few days earlier than the non-irradiated material. Irradiation of sowing mycelium by red light reduces the inoculated amount of mycelium in the substrate at least by two times. The effect of light with a wavelength of 660 nm on the activity of sowing mycelium of two spore mushrooms was investigated. The increase of yield of *Pleurotus ostreatus* was 10% after the irradiation of mycelium.

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Spectroscopy characterization of $Zn_{1-x}Co_xO$ layers prepared by printed electronics method

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Co-doped ZnO films are predicted to belong to promising dilute magnetic semiconductors that may be used in future spintronic devices. The search of new methods for fabricating ZnO:Co with required properties still remains an open question.

$Zn_{0,99}Co_{0,01}O$ layers studied in this work have been synthesized by the improved printed-electronics method patented by the authors. Layer fabrication included paste preparation, its printing on (0001)-sapphire substrates, drying at 130 and 170ºC and crystallization at a temperature about 1000°C.

Studying of layer surface morphology by scanning electron microscopy and atomic force microscopy revealed the polycrystalline nanostructures with a grain diameter from 400 to 600 nm. Registration of (100), (002) and (101) peaks in the X-ray diffraction spectra indicates that the layers have the wurtzite structure without a preferential crystallites orientation. Observation of the E_2(high), E_2(low) and A_1(LO) modes in the Raman spectra also confirms this conclusion. Optical absorption and photoluminescence spectra reveal a band attributed to Co^{2+} interatomic *d–d* transitions associated with the crystal-field splitting in the ZnO host. A broad absorption band at 2.5-3.0 eV observed in optical absorption spectra corresponds to a charge transfer process ($Co^{2+} \rightarrow Co^{1+}$). With increasing the drying temperature of ZnO:Co layers from 130 to 170ºC, the Raman spectra show a significant broadening of the E_2(high) and E_2(low) phonon modes due to a structural disorder associated with the increase of Co content in the layers. Additional vibrational modes observed in the Raman spectra in the range of 530-580 cm^{-1} are explained as disordered Zn-O-Co local vibration modes. These modes are specific to Co doping and haven’t been observed in the undoped ZnO layers. An analysis of the E_2(high) mode in the Raman spectra shows that the magnitude of the elastic strain as well as the structural quality of the layers depend on drying temperature during the layer fabrication.

Device for germicidal disinfection of drinking water

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The results of the physical implementation of nonchemical methods of bactericidal water disinfection by UV irradiation are presented. On the basis of theoretical calculations and experimental data the device for bactericidal inactivation of drinking water has been proposed.

Bactericidal effect of ultraviolet radiation acts on the wavelength range of 205-315 nm [1]. The most effective impact energy of UV radiation from germicidal perspective occurs at a wavelength of 253.7 nm.

The purpose of the proposed technical solution is to simplify the design and reduce maintenance costs while maintaining the efficiency of disinfection of water.

In the known structures devices of productivity and the size of the Rays camera calculated by standard methods using the experimentally determined volumetric dose to inactivate various types of microorganisms H_V . The disadvantage of this approach is that the volume dose H_V depends on the geometry of the camera for exposure and degree of mixing water during irradiation in laminar flow. To obtain the required dose of disinfection H_S , the size of the camera for radiation (diameter and length) should provide the required minimum radiation $E_{\min}$. Other areas will receive "excessive" exposure that only increases the reliability of disinfection.

The required dose H_S (W·cm^2) is achieved variation $E_{\min}$ (W·m^2) or time t(s): $H_S = E_{\min} \cdot t$.

The principle of operation of the device for germicidal disinfection of drinking water based on the following - $E_{\min}$ is calculated from the condition: $H_S \geq 100 \frac{m \cdot J}{cm^2}$.

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Inverse Raman scattering in ultrafast pump-probe experiments

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Inverse Raman scattering (IRS) is a form of nonlinear Raman scattering first mentioned in 1964 [1]. This effect is very briefly mentioned in traditional Raman spectroscopy handbooks due to its complexity. When a medium is irradiated with intense laser light ν_L and continuum at higher frequencies, absorption occurs in continuum at frequencies $\nu_L+\nu_R$, where ν_R is Raman frequency of the medium. Meanwhile this method allows to deliver new possibilities to traditional Raman spectroscopy, like measurement of Raman spectra in gases and diluted solutions and time resolved Raman spectroscopy of excited systems.

In this paper IRS of water and decane solutions during femtosecond pump–white continuum probe experiments are shown. Due to significant spectral width of the pump pulse (10 nm for 150 fs pulse duration), IRS does not provide fine spectral resolution, but it has hundreds of femtoseconds temporal resolution.

We used Ti:Sapphire femtosecond laser with regenerative amplifier which produce laser pulses with 800 nm wavelength, 1 mJ pulse energy at 1 kHz repetition rate. In order to produce white light continuum, laser was focused into 1mm thick sapphire plate. White continuum spectrum ranges from 400 nm to 1000 nm. Probe pulse was spatially and temporally overlapped on the sample with a pump pulse. Induced absorption of the sample represents IRS spectra.

Measurements were performed at the Center for collective use of the Femtosecond Laser Complex of the National Academy of Sciences of Ukraine.

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Stimulated Raman Scattering of dyes in scattering cover

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Coupling of stimulated Raman scattering (SRS) and random lasing (RL) of dyes in multiple scattering media (MSM) reveals all their Stokes lines in RL spectrum what may be applied to studing of Raman spectrum. However, fabrication of proper MSM is impossible when scattering particles are incorporated into medium because of their interaction with the dye causing its bleaching. This problem may be solved with "photon box" (PhB) which is sample enclosed in scattering cover of high reflectivity. Placing of scattering centers only on the sample surface practically excludes the bleaching. In contrast to bulk MSM multiple scattering in PhB occurs on the sample surface.

We studied radiation of Rhodamine 6G, Polymethene 920 and Pyrromethene 605 in PhB with internal part of dyed olihouretan acrylate and outer scattering cover made of concentrated suspension of borazon microparticles. We observed SRS lines of all dyes on continuous background of their RL spectra, which are similar to spectra of dyes radiation in bulk MSM. Behaviour and dependence of the PhB radiation spectrum on pump intensity is similar to the same characteristic of radiation in bulk MSM. This similarity testifies to occurrence of SRS and RL in PhB. Effectivity of their manifastation depends on ratio of the volumes of inner part and active zone of the sample. It appears via threshold pump decrease and SRS line contrast groth under volume ratio decrease.

The best manifastation of SRS and RL effects in PhB was observed in Polymethene 920 in which most intensive and sharp lines were revealed. Fabrication of bulk MSM such as concentrated suspension of rutil microparticles and vesicular films is impossible because of the bleaching. Thus, obtained results demonstrate that PhB may be considered as alternative MSM acceptable for Raman spectroscopy application. For SRS facilitation, one should apply PhB of minimal relative volume.

Plasma assisted combustion of stearine pretreated by magnetic field

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The idea of using nonequilibrium low-temperature plasma for ignition or combustion stabilization is among the most promising areas of modern plasma-chemistry. There is a number of papers devoted to reviewing the research of different gas discharges, which are used for plasma-assisted ignition and combustion. In addition, different mechanisms for such phenomena as ion chemistry and chemistry of excited species are proposed and investigated.

The combustion of high viscosity hydrocarbons is obstructed due to their inefficient atomization. Traditional gas-dynamic jets are not suitable solution for this problem. Therefore, the creation of new plasma-liquid systems that would allow effective atomization of high viscosity hydrocarbons is an important and promising direction for investigation. This work concerns the plasma-assisted combustion of high viscosity hydrocarbons. Plasma jet was used for the atomization of high viscosity hydrocarbons. The stearine in solid state, which was pretreated in melted state by magnetic field of varying strength (0-2.4 mTl), is used as the model of solid paraffin-based fuel. Rotating gliding discharge was used as a plasma source. This type of systems can be used for generation of non-equilibrium plasma. Plasma system consisted of the plasma formation area, the area where plasma was injected and interacted with hydrocarbons, and the flame area.

The current-voltage characteristics of the rotating gliding discharge were measured. The diagnostics of plasma torch and flame were carried out via emission spectroscopy. The temperature of flame generated during plasma-assisted combustion of hydrocarbons was measured.

This system provides the maximum contact between plasma and hydrocarbons, thus allowing plasma to be simultaneously used for the stimulation of stearin phase transitions from solid to aerosol/vapor form, partial conversion of stearine into synthesis gas and support of complete oxidation (combustion) processes.

Iterative evaluation of vibrational spectra of dyes from their SRS-SE spectra

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In a multiple scattering medium (MSM) stimulated emission (SE) and stimulated Raman scattering (SRS) of dyes interact forming integrated nonlinear process (SRS-SE) with joint emission spectrum [1]. It gives a possibility to evaluate the corresponding section of the molecule's vibrational spectrum (VS). In order to calculate VS, background subtraction procedure should be done very accurately.

There are many different background subtraction techniques based on polynomial fitting [2], discrete Fourier transform, or wavelet transform etc. However, all these techniques have one joint drawback: they do not account for properties and nature of this physical process.

A new technique of estimating VS from the SRS-SE spectra is presented. Our technique consists in simultaneous processing of a batch of SRS-SE spectra received under different experimental conditions. The proposed method uses the conception of VS independence on experimental conditions such as pump intensity or concentration of dye molecules. It means that VS calculated from the decomposed SRS-SE spectrum must be the same for every spectrum from the batch. Thus, the proposed method iteratively minimizes the residual between VS. Initial background's subtraction is done individually for each spectrum with a method similar to [2] but using a sum of two Gaussians as a fitting function.

The proposed technique was tested with laser dye pyrromethene 597. Diminishing of the residual between the vibrational spectra was used as a quality criterion. Matching between the received spectrum and a vibrational spectrum computed with Gaussian 09 software was used as an adequacy criterion. It was shown that our method could distinguish weak vibrational lines that could be interpreted as a noise in individually taken spectrum.

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The using of magnetic field for the improvement of properties of liquid fillers in a liquid lense

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Today in optical-electronic industry the liquid lenses are widely used [1]. These developments much attention is sanctified to. The liquid lens with the function of down-scaling and liquid lenses for an optical-electronic equipment on the basis of water solution of $CaCl_2$ are referred to such type of the liquid lenses. For the improvement of image qualities of liquid lenses at development pay attention to properties of liquid filler for the exception of possibility of chromatic aberration. Necessary to take into account co-operation of the liquid system with a hard surface for deciding this task. As is known between liquid and hard surface the wall layer is formed [2]. It is suggested to use follow liquid fillers. The molecules of such liquid system able under the action of light wave with different length to change the configuration thus, that the size of wall layer remained permanent. The liquid systems with a dipole magnetic moment is proposed for this aim [3, 4].

The 5% glucose water solution with addition to glycerin was investigated at static magnetic field with induction of 0,43mT and without magnetic field. The obtained results showed that at previous treatment in the magnetic field the omission in area of red color folds 98%, in an area of violet color equals 99%. In absence of magnetic-field the omission in area of red color folds 86%, in area of violet color equals 96 % The molecular mechanism of these results is related to the settlement of processes of formation and disintegration of concentration fluctuations of the particles in the liquid system under the action of magnetic field.

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The experimental method for the study of intermolecular interactions in a magnetic field transparent liquid systems

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The problem of structure changes in liquid “water-saccharides” systems due to the changes of interaction character is widely discussed in many works [1]. These works underline that intermolecular interaction change is followed by the change of the viscosity in these solutions [2]. Moreover, there are works, which mark changes of this kind as the result of magnetic field influence on the regarded “water-saccharide” liquid systems.

In order to investigate the aforementioned effect, the method, based on the Stokes method, is proposed. The benefits of the proposed experimental method include the possibility of usage of small volumes of the regarded substance, the extended range of viscosity measurements and the ergonomics of the experimental facility.

The schematics of experimental facility is given at Fig. 1.

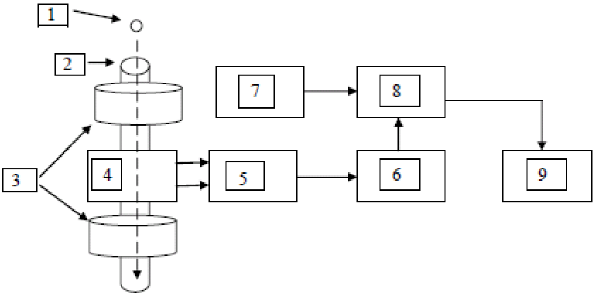

Fig.1. Experimental facility schematics (1 – glass ball; 2 – glass cylindrical cuvette with the regarded system; 3 – windings of electromagnet; 4 – monoblock, containing two pairs light emitting diode (LED) – phototransistor (ФТ). Each pair LED and PT are placed in the apertures of monoblock one against another, and the measuring beam is registered on the other side by PT after passage through the cuvette. The distance between upper and lower pairs of LED-PT is 2 cm; 5 – scheme for impulse-formation, which turn on the trigger 6; 7 – impulse generator with the frequency of 1 kHz. These impulses are submitted through the electronic key to the scheme 9 – the counter of impulses with the light emitting diode seven – segment indicators. The maximal number of impulses is 1000).

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Application of videopolarimeter for evaluation of chiral homogeneity of aqueous solutions of optically active substances

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Evaluation of chiral purity of pharmaceutical drugs is a very urgent task, since the presence of chemically identical therapeutic substances, but with mirror opposite molecular structure, often leads to adverse effects of drugs using.

In nature, generally, one or another molecular form prevails, but artificially synthesized substances usually contain a mixture of enantiomers, which are absorbed differently by the body. Today only about 15% of synthetic drugs are tested on chiral homogeneity; other 85% are potentially dangerous mixture of isomers.

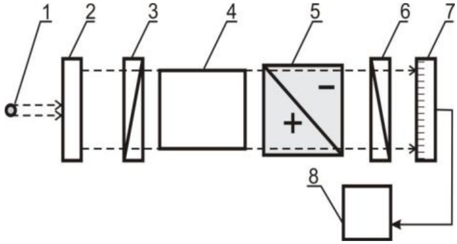
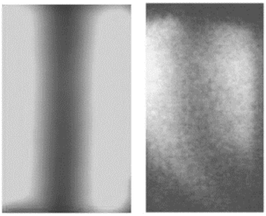


Fig. 1. Block diagram of video polarimeter: 1-light source, 2-extender of beam of light, 3-polarizer, 4-sample cell with investigated optically active material, 5-spatial modulator, 6-analyzer, 7-matrix photodetector, connected to 8-computer interface.



a b

Fig. 2. The spatial intensity distribution at the output of the analyzer for glucose solution (a), and for the drug solution "Inulin-nutrymed" (b)

Development of methods for water activation and a study of optical and physical properties of metastable aqueous solutions

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The deterioration of health is associated with deficiency of electrons in the environment and drinking water. Deficiency of charge particles association promotes blood - thus triggers blood clotting and strokes, creating problems of cell metabolism. Molecules - antioxidants have one free electron that they give, and thus protect cells.

One of the most valuable suppliers of antioxidants is water, which is negative oxidation-reduction potential (ORP). One way of providing such properties are water enrichment of hydroxyl ions OH^-. On the other hand excess protons H^+ in water inhibits the biological processes that allows the use of protonated water as a means of combating pathogens.

We suggested methods and devices for the transfer of water solutions in metastable state under the influence of electromagnetic fields and got metastable aqueous solutions, which for a long time (several days) coexist existing active substances in conventional aqueous mutually neutralized within minutes. It is possible to obtain aqueous solutions with different ORP in the range from -600 mV to +900 mV and a constant pH value (pH~7.7-8.2) characteristic of plain water.

Because metastability such solutions do not accumulate in the environment that causes their environmental safety and eliminates the possibility of addiction microorganisms to antiseptics such. Low total mineralization (average 3 g / l) closer to the antiseptic properties of normal or weakly mineralized water. Low concentration of active ingredients (about 0.3 g/l) makes our antiseptic secure in contact with skin and mucous membranes.

Design feature allows the non-equilibrium solutions in vessels of different shapes and volume, does not require additional devices (pumps, diaphragms, etc.). Possible to use autonomous sources of electric power with different voltages, such as a battery voltage from 6V to 24V.

In the process of establishing equilibrium aqueous solutions under the influence of electric and magnetic field changes the structure of water cluster, which may be to change the viscosity of water. The viscosity of water is selected as the sensor impact of electric or magnetic field. Particular attention is paid to temperature control during measurement to exclude the impact of this factor on the results of experiments. The algorithm ensures data accuracy temperature 0,010S order. For natural water, pH=6.65, ORP=289 mV after activation of membrane electrolyzer obtained pH=8.86 and ORP=52 mV (for catholyte). The relative viscosity changed between 1 and 1.0877±0.0007, the viscosity is increased by 8.77%.

The design made viscometer also allows us to measure changes small-angle laser scattering in water (in the range ± 6 deg.). We carried out successful test of the proposed testing technique of digital registration of the intensity distribution in the cross section of the probe radiation and algorithm processing of the results. This will allow in the future to explore the relationship between the change in the viscosity of water and its structure in external electric and magnetic fields.

Generation of antioxidant water and its properties analysis

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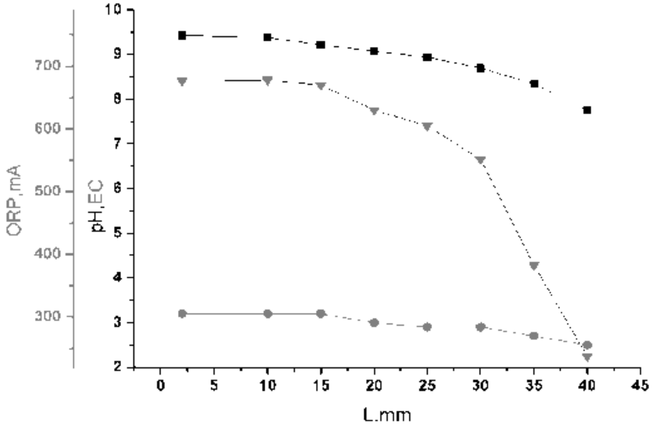
In our research, we consider antioxidant water that has a negative Redox potential. It allows the human body to neutralize free radicals, prevent it from premature aging and reduce the risk of many diseases. Consuming this water human body receives the necessary electrons and "restoring" increases the immunity of the organism. There is no alternative method of obtaining weak alkali water with antioxidant properties except for using devices based on electro-chemical activation. (EChA). This report contains describing methods and devices, which are used to obtain this type of water.



Anolyte means a water solution obtained in the small container of the device. The people called it "dead water", but it has, on the contrary, a high acidity and high redox potential. Thanks to these characteristics, the anolyte has a pronounced antibacterial properties and powerful antiseptic, analgesic, anti-allergic action. It is effective for disinfection (including salmonella cholera, dysentery), angina and chronic tonsillitis. It is used in surgery as an antiseptic agent for the treatment of festering wounds, abscesses, phlegmons, etc. The anolyte is also successfully applied in treatment of burns, bedsores and other skin diseases. The liquid is colorless, but has a faint smell of chloride. The anolyte is relatively resistant, does not lose its activity within 7 days. Must be stored in a dark place in a tightly closed container. Anolyte can be prepared in the boiled or not boiled tap water for outdoor use.

Peculiarities of the temperature dependences of oxidation-reduction potential (ORP) water

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Increased interest in studying ways to obtain water and aqueous solutions with negative values of the oxidation-reduction potential (ORP) because the activity of electrons is the most important characteristic of the internal environment as directly related to the fundamental processes. Normally ORP internal environment of the human usually ranges from "-" 100 to "-" 200 mV, that is recovery state. ORP ordinary drinking water (water from the tap, bottled drinking water, etc.) usually has positive potential of "+" 200mV to "+" 300mV and when this water gets into human tissue, the biological structure (cell membranes, nucleic acid) are subjected to acid degradation. These negative processes can be slowed if drinking the water that has properties similar to those of the internal environment, i.e. renewable protective properties. Of course, such useful properties of water associated with its enrichment hydroxyl ions OH-. This stimulates biological processes - Seminal similarities, their germination and plant growth, cell division in animals. Such hydroxylated water getting into the human body, cells and tissues enriches electrons, which dramatically increases the electron-proton transport, underlying the metabolism. Increases the rate of ATP synthesis, proteins, nucleic acids and other cell components. Conversely, excess protons H + inhibits biological processes. In protonated water (pH~ 5,5) decreases fluidity of cell membranes, membrane proteins are collected in clusters, leading to the suspension of metabolic processes in cells and tissues. Normally such a condition occurs before cell division when the cells of virtually off-exchange processes. Moreover, the enrichment of water hydroxyl ions OH- membrane of normal cells are activated, they amplified metabolism. This phenomenon is called natural doping. Enrichment of water OH inhibits cancer cell division. Perhaps the mechanism underlying the anti-cancer action of such water. There is a version that enhances the ability hydroxylated water metabolism because the same membrane OH- ions repel each other, promoting the opening of membrane channels for micro and trace elements and other compounds involved in metabolic processes. Unfortunately, stability hydroxylated water is negligible. Water in such a nonequilibrium state returns to the original for two - three days. In addition, there is a need of biologically active liquids (water solutions) with a negative ORP at different temperatures.

We have developed several methods and devices for obtaining a water and aqueous solutions with negative ORP, rated their ability to apply for medicine (e.g., photodynamic therapy, to create means to prevent the concentration of blood clots, etc.).

An interesting for practical application is, in our opinion, the method of cooking water in a nonequilibrium state with the same pH, but with significant changes ORP (from "+" to 300mV "-" 500mV.)

Investigated the impact of technology nonequilibrium cooking water with negative ORP ORP Depending on the temperature and temporal stability of parameters.

Analytical role of Raman spectra

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Application of Raman scattering for analytical purposes is because the Raman spectrum is an individual optical characteristic of a molecule. Due to this, the Raman spectrum can be used for reliably identification of scattering molecules. Often, one can set in the spectrum some group characteristics that are typical for a class of compounds.

Recently, there was an interest in developing gas analyzers of natural gas (NG), based on the use of spectroscopy of spontaneous Raman scattering (RS). This method allows one simultaneously and with high accuracy to determine the concentration of actually all molecular components of NG [1].

The paper presents an investigation of Raman spectra of natural gas (NG). Research was carried out on an automated spectral setup DFS-52 modified for the purposes of the experiments. The excitation source was argon laser LGN-503 with the wavelength of 488.0 nm and the output power of 1W.

In the natural gas the most intense Raman spectrum is observed in the region of combination frequencies 2500-3300 cm^{-1}, where the system of vibrational bands ($\nu_1(A_1)$, $\nu_3(F_2)$, $2\nu_2(A_1)$, $(\nu_2+\nu_4)(F_1+F_2)$, $2\nu_4(A_1)$) of methane is located having a complex rotational structure. Thus, we have two valence vibrations ν_1 and ν_3 of symmetry A_1 and F_2 and two deformation vibrations ν_2 and ν_4 of symmetry E and F_2. These vibrations are active in the Raman spectrum. In the Raman spectrum, along with three degenerate frequency ν_3 we observed only symmetric valence frequency ν_1=2916,5 cm^{-1}. In the same region of the spectrum, there are bands of stretching vibrations of C–H bonds and all the heavier hydrocarbons of the natural gas. In this complex system of bands there is released a very intense Q-branch of the vibrational band ν_1 of methane with frequency 2916.5 cm^{-1} [2].

The results show that for the analysis of component composition of NG is suitable low frequency (500-2000 cm^{-1}) sides of the Raman spectrum, where are located the vibrational bands corresponding to stretching vibrations C–C-bonds of hydrocarbon components of NG.

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Ranging by frequency-shifted feedback diode lasers: the consequences of spatial inhomogeneity effects

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Frequency shifted feedback (FSF) lasers have been demonstrated to be powerfull tool for very precise measurement of distance. The use of a phase-modulated seed to the FSF laser dramatically improves the accuracy up to expected of optical interferometry.

We present a detailed analysis of the consequences of spatial inhomogeneity of laser profile and surface structure for ranging with FSF laser. We derive an analytical expression for the ranging signal in the case of phase-modulated seed and analyze it for several special cases. In particular, we consider the step-like mirror object and show that interference influences the step resolution. We also show that the superposition of the contributions from different parts of an illuminated titled surface leads to a substantial decrease of the signal amplitude.

We analysed the possibility of using of adaptive interferometry approach to minimize the influence of the spatial inhomogeneity on the accuracy of the ranging by FSF lasers.

Absorption and luminescence spectra of natural dyes in catholyte aqueous solutions

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Recently there has been increased interest in the so-called photodynamic therapy (PDT) of cancer. Successful application of PDT is largely dependent on the characteristics of the absorption and luminescence spectra of dyes. Very acute is the question of creation of dye solution in liquids whose parameters are close to those of human biological liquids, as otherwise the use of dye solution in itself creates a health hazard.

The work describes several ways of making dyes and comparison of their absorption and luminescence spectra. Of particular interest are solutions prepared from catholyte ("traditional" catholyte, which altered pH and redox potential (ORP) and catholyte with variable ORP and constant pH). As known catholyte has increased extracted possibility compared to the anolyte and water and so it was interesting to compare the properties of "traditional" catholyte and catholyte as a new type of solvents by measuring their absorption spectra.

On the other hand, measuring and comparing luminescence spectra of dyes prepared in that way provide important information about their suitability for the stimulation of singlet oxygen emission. We assembled a digital spectrograph which allows one to quickly obtain absorption and luminescence spectra in the range from 400 to 800 nm.

Optimization semiconductor laser to excite luminescence

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Recently there has been a growing trend to use semiconductor lasers in scientific research, particularly in biophysics and medicine. The problems related to the stability of the spectrum and intensity of radiation in general, are very difficult to be solved. Typically, allocation green spectral line λ = 546 nm is traditionally used from mercury lamp spectrum, which results in a complex scheme of stabilization, lamp ignition and cooling. When using semiconductor laser instead the mercury lamp we have a problem with absence of monochromatic light. Typically, the halfwidth of the spectral line of green laser is more than ten nanometers, so it is not convinient to excite the biological objects.

To solve this problem, it is possible to create the conditions in which the semiconductor laser emits stable and a radiated line halfwidth is aboutseveral nanometers. Mostly, the spectrum of the laser radiation affects the temperature of the semiconductor junction. This in turn should affectconsequence of current through the p-n junction. Therefore, it would be rational to analyze the change in emission spectrum depending on these two factors.

As an investigational semiconductor laser was used green laser pointer with a wavelength λ = 532 nm spectral line width Δλ which is 1-2 nm depending on the duration of exploitation. The longer operates the device, the more the temperature it has. As a result, it has two or three unstable spectral lines (occasionally with unstable wavelength). So to get a single-line in the spectrum it`s necessary to cool the p-n junction and reduce its current supply.

Experimentally found that to achieve the effect of temperature should be close to 270 K, and the current should not be greater than 50mA. It was therefore replaced the laser housing to increase the absorption capacity of the radiator. The temperature radiator was controlled by Pelt'ye's elements.

This method allows relatively simply and effectively get a stable and narrow spectral line.

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7

Molecules

Femtosecond transient absorption spectroscopy of new two-photon absorbing fluorene-containing quinolizinium cations

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The linear photophysical characterization, and nonlinear optical properties of two new symmetrical fluorene-containing quinolizinium derivatives, 2,8-bis((E)-2-(7-(diphenylamino)-9,9-dihexyl-9H-fluoren-2-yl)vinyl)quinolizinium hexafluorophosphate (**1**) and 2,8-bis((E)-2-(7-((7(diphenylamino)-9,9-dihexyl-9H-fluoren-2-yl)ethynyl)-9,9-dihexyl-9H-fluoren-2yl)vinyl)quinolizinium hexafluoro-phosphate (**2**), are reported. The nature of the dual-band steady-state fluorescence emission of **1** and **2** was determined, and violation of Kasha's rule along with a strong dependence on solvent polarity was shown. A relatively complex structure of two-photon absorption (2PA) spectra of **1** and **2**, with maximum cross sections of ~ 400-600 GM, was determined using the open aperture Z-scan method. Different types of fast relaxation processes with characteristic times of 0.3 - 0.5 ps and 1.5 - 2 ps were observed in the excited states of the new compounds via femtosecond transient absorption pump-probe spectroscopy technique. A potential application of new fluorene-containing quinolizinium derivatives in laser scanning fluorescence microscopy was demonstrated via cell membrane fluorescence imaging of HeLa cells.

MCR-ALS analysis of multicomponent liquid solutions in Raman and FTIR spectroscopy

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Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS) [1,2] method was used for the determination of spectra and concentrations of species in multicomponent (up to 8) liquid solutions by analyzing Mid-IR, Near-IR and Raman spectra.

It was shown that MCR-ALS can be successfully applied to resolve spectra and concentration profiles when number of species is low. If the number of components N is higher than four or five, MCR-ALS technique fails to resolve similar components properly. But if the object under investigation has components with known vibrational spectra, they can be used in MCR-ALS as fixed values in rows of a matrix of spectra “S”. Such procedure can be viewed as a hybrid technique for decomposition using library spectra and MCR analysis. This way MCR can be applied to the mixture of more than 20 components where $N-5$ of them are known. As the result one can obtain spectra and concentration profiles of remaining unknown species.

In the case of Raman microscopy, the effective number of components in the mixture of N compounds should be increased to $N+2$. One of the additional components represents fluorescence background, and another additional component describes contribution of microscope objective and cover glass to Raman spectrum. Introducing these additional components to MCR analysis allows separating unwanted additives and helps to increase the accuracy of quantitative analysis of concentrations in multicomponent solutions.

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Glaciation process in triphenyl phosphite investigated by infrared spectroscopy

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Triphenyl phosphite (TPP) is well known to exhibit an intriguing transformation of the supercooled liquid [1]. If TPP is cooled rapidly enough, it first enters into a supercooled liquid state below the melting point *Tm* (~299 K) as usual liquids, and then into a glass state at the glass-transition temperature *Tg* (~210 K). On the other hand, if TPP is quenched to a certain temperature between 212 and 225 K (above *Tg*) and then annealed at that temperature, a new phase (the so-called “glacial” phase) emerges in a supercooled liquid and growth with time. The transformation to the glacial phase was named as “glaciation”. However, the structural configuration of the “glacial state” remains an open question, therefore the determination of the nature of the “glacial state” is of great scientific interest.

In order to get a better insight into the nature of the glacial phase in TPP, we have carried out *in situ* IR spectroscopic investigation of the structural changes during the glaciation process at 215, 218 and 220 K in TPP, which allows analyzing in real time the structural evolution of TPP. Infrared measurements were done on a Fourier-transform infrared (FT-IR) spectrometer (Bruker model IFS-88) at a resolution 2 cm^{-1} in the 400 – 4000 cm^{-1} spectral range. According to our IR spectroscopic results, we interpret the glacial phase as composed of nuclei of the stable phase, characterized by a size strongly dependent on the aging temperature in the matrix of an extremely viscous liquid, which is not an ordinary supercooled liquid.

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Hydrogen-bonded clusters in molecular liquids

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The processes of molecular cluster formation in monohydric alcohols were investigated using FTIR spectroscopy and a matrix isolation technique [1-4]. The methods of cluster isolation in low-temperature matrices provide the possibility to study individual clusters of different sizes. FTIR spectra of monohydric alcohols (from methanol to decanol) in argon and nitrogen matrices were registered in the frequency range from 500 cm^{-1} to 4000 cm^{-1}. The gradual transformation of the spectral bands assigned to different vibrations was observed with matrix heating from 10 to 50 K, indicating a transformation of the structure of the isolated clusters. Main changes with the temperature increasing were observed in the spectral regions of stretch O-H and C-O vibrations.

The observed temperature dependence of the registered spectra may be considered as a model of structural transformations in alcohols during the phase transition from gas to liquid state.

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Temperature evolution of cluster structures in 1-nonanol

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In this work, our research group present new results of temperature evolution investigation of cluster structure in 1-nonanol. The 1-nonanol molecules are much bigger than methanol and there is no such an amount of information and publications about it.

Investigations of alcohols and their cluster structures are very popular and we can see such an amount of papers with results of research on this field in different scientific journals. Many authors have focused on investigations of the simplest alcohols like methanol and ethanol, because there is a possibility to apply such types of investigations as experimental and theoretical technics. There are only six atoms in methanol molecule and this fact allows authors to use different experimental technics like matrix isolation or isolation in helium droplets for example. Modelling calculations for substance like methanol and ethanol are simpler in comparison with analogue calculation for molecules with bigger number of atoms. Experimental and theoretical investigations of 1-nonanol are more difficult than analogue ones. That is why 1-nonanol is an object of our research.

We use FTIR spectra method in region from 500 cm^{-1} to 4000 cm^{-1} at temperature from -20 ^{o}C to 0 ^{o}C. The comparison of the registered IR spectra at temperature near phase transition allows us to understand how many varied clusters we have before and after phase transition. The spectral regions of O-H and C-O bonds are especially interesting and informative. Spectral changes in those vibration regions demonstrate us structure transformation from smaller cluster to bigger in process of phase transition.

Water molecules investigation

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There is such an amount of works and discussions about what is water structure, why it is such and so on. These discussions did not subside for many years and even in our age of discoveries in various fields of science, we cannot say exactly, what it is, why it is and how it is.

We have investigated different alcohols and structures with one hydrogen bond to understand interactions between them. After going through the entire series from methanol to decanol we start to research water molecules.

Those fact, that water molecule consists less atoms then any simple alcohol (for example, methanol), assume that we have more possibilities for investigate, as experimental, as theoretical and computational (ab initio, MD, etc). However, the simplicity is deceptive. Two hydrogen bonds in water greatly complicate calculations of water molecules clusterisation. It results in bigger variety of molecules states and makes experimental data interpretation and comparison with theoretical calculations much more difficult.

This work represents our attempt to calculate and understand structure of water in different conditions using various methods to find out what is the reason for strange and abnormal water behavior. We have used different techniques to get FTIR model spectra. Large amount of experimental data (spectra in condensed phase, in matrix isolation) allows us to analyze our calculations more correctly due to the fact, that experimental data is the only way to check the probability of existence in real life such results of combining theoretical approximations, our ideas and computational systems.

This small molecule is fraught with as many more secrets to uncover!

Quantum-chemically study of interaction between fullerene and covalent bonded pentamethinecyanine

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The fullerenes C_{60} have attracted a great deal of interest because of their unique structure and properties. Amound fullerenes derivatives, the C_{60} molecule with the covalent linking conjugated systems (for example, porphyrins, phthalocyanines or perylenes), which can be light harvesting antennas and electron donors should consider as the perspective. Using of conjugated systems absorbing in UV/visible region enables to investigate the interaction between π-electrons of the fullerenes and linked molecule by spectral methods. The polymethine dyes with their high intensive and selective absorption are excellent convenient objects for such study.

Presented work deals with study electron structure and molecular geometry of the composite molecule containing the fullerene and chemically bounded indopentamethinecyanine by quantum-chemically and spectral methods.

Quantum-chemical calculation of optimized molecular geometry were performed by HF/6-31(d,p) and DFT/CAM-B3LYP//6-31(d,p) methods; the electron transition characteristics were calculated by the non-empirical (TD/DFT/6-31G(d,p)/CAM-B3LYP) method and semi-empirical ZINDO method in the package CAUSSIAN 03.

It is shown that the new synthesized molecule absorbs in both in UV and VIS regions, has singlet and triplet transitions that makes it perspective in use in the photodynamic therapy.

Some notes on weak complex OC-HF formation based on FTIR gas phase spectrum

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In this work, the gas phase spectra of hydrogen fluoride (HF) and carbon oxide (CO) mixtures were investigated using Fourier transform infrared (FTIR) broadband spectroscopy technique for the region from 3838 to 3854 cm^{-1}. The OC--HF complex bands that can correspond to the excited intermolecular (complex) stretching and bending, were observed at different densities of OC component and fixed HF component. The observed hot bands were assigned with the help of the fitted spectra for slightly non-rigid linear molecule. The problem of correct interpretation of the obtained data is raised through the modeling potential energy of the “weak” interaction. We discuss the possibility to estimate the corresponding potential barrier allowing the components to be coupled for a relatively long time in comparison with just collision time, when the corresponding energy surface does not possess a local maximum above "zero" level with respect to distance between the monomers. Therefore, the question is about the processes that "make the complex happened". Hence, if reverse polarization is neglected when dealing with the semi-classical model potential including attractive dipole-dipole interaction between the monomers, such kind of hydrogen bonding potential should have significant enough contributions from rotationally “excited” distortion energy and/or the item of ionic interaction.

Molecular complexes formation in binary liquid solution of benzene with chloroform

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The molecular complexes formation in liquid benzene-chloroform solution was investigated by infrared spectroscopy techniques. The multivariate curve resolution (MCR) techniques [1] were used for evaluation of quantitative information about mixture components.

MCR methods are based on bilinear model:

$$\mathbf{D}=\mathbf{C}\mathbf{S}^{\mathbf{T}}+\mathbf{E} \qquad (1)$$

The goal of MCR-ALS is the bilinear decomposition of the data matrix **D** into the "true" pure response profiles associated with variation of each contribution in the row and the column directions, represented by matrices **C** (which contains components concentration) and $\mathbf{S}^{\mathbf{T}}$ (which contains components spectra). In spectroscopic measurements, the rows of matrix **D** are the spectra (measured during the experiment); **E** is the matrix of residuals which are not explained by the model and in ideal case should be close to the experimental error.

In general, MCR problem (1) doesn't lead to unique solutions only. Non-linear constrained optimization methods are often used for recovering band boundaries of feasible solutions [2]. Model-based approaches also can be used for decomposition of matrix **D** [3].

Both model-free and model-based approaches for decomposition IR spectra of liquid benzene-chloroform were used. We concluded that spectrum of the mixture can be described with high accuracy as a linear combination of spectra of three components: pure components (unbounded benzene and chloroform) and molecular complex.

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Photophysical studies of the derivatives of carbazole and tetra(tri)phenylethylene with aggregation-induced emission effect for organic electroluminescent devices

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We report on luminescent and electroluminescent properties of new derivatives of tri- and tetraphenylethylene and carbazole with strong blue luminescence and aggregation-induced emission (AIE) effect. For the estimation of AIE activity of the new compounds the fluorescent behavior of their dilute solutions in the mixture of THF and water with the different water fractions were studied. The emission of the THF solutions of the studied derivatives was weak, however, a dramatic enhancement in luminescence intensity was observed for the 60:40 (v/v) water/THF mixture. Since these derivatives are insoluble in water, the increase of the water fraction in the mixture of solvent leads to the reduction of the number of the dissolved molecules of the compounds. After reaching the certain ratio of water and THF (ca 50:50 v/v) the molecular aggregation starts to occur in the mixture of solvents, which leads to the enhancement of the emission. Taking in account the strong blue emission and AIE, we used these carbazole and tetra(tri)phenylethylene derivatives and 4,4′,4″-tris[3-methylphenyl(phenyl)amino] triphenylamine (m-MTDATA) for the preparation of organic light-emitting diodes the electroluminescence spectra of which include exciton and exciplex emissions. The low-energy exciplex emission band of the electroluminescence spectra was formed at the interface of the emissive layers. The best fabricated device showed values of a turn-on voltage 2.7 V for electroluminescence (at 10 cd/m^2); maximum current efficiency of 11.5 cd/A, maximum brightness of 17700 cd/m^2 (at 11 V), and external quantum efficiency of ca. 3.9 % with CIE 1931 chromaticity coordinates (0.20, 0.38).

Low-power optical irradiation influence on alcohols droplets evaporation processes

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In the report, the experimental data according alcohols (n-propanol, n-butanol, n-pentanol, n-heptanol, n-octanol and n-decanol) droplets evaporation into gas-vapor mixture of droplet substance's vapor and buffer gas under optical irradiation influence were considered. The experimental results were received for the nitrogen buffer gas pressure values 30, 50, 100, 200, 400 mm Hg and low-power (0.1 W) irradiation with wavelengths 390, 590 and 680 nm.

The measurements were carried out using the method, described in [1]. Experimental evaporation rate values were calculated from droplet's size dependence on time obtained by processing droplet's images. These images were received by using special camera, recording droplet in certain time interval. The droplets were hanged in working chamber at special suspension (chip transistor) allowing also to measure droplet's temperature with accuracy about 0.03 K. The values for the alcohols evaporation rate were calculated in the dark regime (without irradiation) as well as under the irradiation influence.

It was obtained the increasing of evaporation rate for the following alcohols: 1-heptanol (37%), 1-octanol (36%) and 1-decanol (85%) under the influence of irradiation with wavelength 390 nm for buffer gas pressure value 100 mm Hg. There are no evaporation rate increasing for alcohols with a small molar mass (1-propanol, 1-butanol and 1-pentanol. It was shown that alcohols droplets heating under irradiation could not cause such increase of the alcohols evaporation rate.

There is no n-heptanol droplets evaporation rate increasing under irradiation with wavelengths λ=590 and λ=680 nm, while behavior of n-octanol and n-decanol is similar like under irradiation with wavelengths λ= 390 nm.

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Diffusion and self-aggregation in long-chain ionic liquids: pulsed-field gradient NMR study

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Diffusion and self-aggregation (micellization) processes in the neat room temperature ionic liquid (RTIL) 1-decyl-3-methyl-imidazolium chloride ([C_{10}mim][Cl]) and in its aqueous solutions have been studied using pulsed-field gradient ^{1}H NMR spectroscopy. The temperature dependences of diffusion coefficients in the neat [C_{10}mim][Cl] perfectly obey Arrhenius-type behavior. This finding has been discussed in terms of the classification of compounds into of 'fragile'-, 'intermediate'- and 'strong glass formers', and that many of RTILs show fragile or intermediate behavior. The presence of the long and flexible alkyl chains, which soften the systems making them less 'fragile'. The obtained value $E_a = 63 \pm 2$ kJ/mol in [C_{10}mim][Cl] gets within those of 21 - 43 kJ/mol for some 'shorter' imidazolium- and pyrrolidinium-based RTILs and 58 - 95 kJ/mol for some long-chain fatty acids (e.g. 4-*n*-penthylcyclohexane acetic, heptadecanoic (C_{17}), nonadecanoic (C_{19}), *etc*) [1].

It can be concluded that the diffusion processes in the neat long-chain RTILs, similarly to other long-chain molecular systems with orientational disorder, go through the cavities (vacancies) and the boundaries of highly dynamic mesoscopic structures.

The critical aggregation concentration $CAC = (1.15 \pm 0.01)\cdot 10^{-3}$ mole fraction and the aggregation number $N_{agg} = 34 \pm 7$ determined from the dependence of diffusion coefficient on concentration in aqueous solution are consistent with the literature data on micelle parameters in closely related systems obtained by small-angle neutron scattering (SANS), conductivity and other techniques.

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Clustering of water molecules: matrix isolation FTIR/2DCOR study and the concept of combinatorial band broadening

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The FTIR spectra of water in argon matrix have been measured while heating the sample from T = 9 K with steps of 2K to 50 K. The main attention has been focused to the spectral range of O–H stretching vibrations at 3000-3700 cm^{-1}. 2D correlation (2DCOR) analysis of FTIR spectra [1] and the non-linear band shape fitting have been carried out. The peaks of monomer up to the higher H-bond clusters (hexamers) have been resolved and analyzed. The results have been compared with the data on water clustering in hydrophobic solvents [2].

The full widths at half height (FWHH) for each band have been processed as the function of the number H-bonds in the cluster and temperature. The combinatorial broadening has been proposed to be the most reliable factor forming diffuse O–H stretching bands in H-bond clusters at these conditions. The combinatorial technique being like based on the entropy consideration can be a promising tool recognizing the vibrational modes in H-bond clusters and correctly them attributing to the proper structures. This treatment can be considered as complementary to the conventional solving of vibrational problem by means of quantum chemistry calculations, i.e. the method that is based on the optimization of parameters using the energy as criterion.

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Spectral characteristics of novel fluorophores synthesized from citric acid

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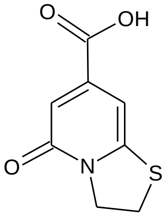
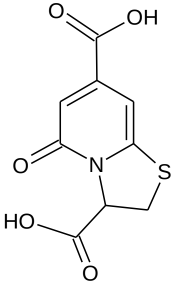


CCA



TPA

A spectroscopic investigation of the electronic structure of novel fluorophores synthesized from citric acid was performed using absorption, fluorescence and phosphorescence techniques.

Fluorescent materials synthesized from renewable resources have gained great attention mainly because of low costs of their synthesis and high quantum efficiency. Two novel fluorescent compounds were isolated from condensation mixtures of citric acid and specific β-amines. Synthesis of 5-oxo-2,3-dihydro-5H-[1,3]thiazolo[3,2-a]pyridine-3,7-dicarboxylic acid (TPA) and 5-oxo-2,3-dihydro-5H-[1,3]thiazolo[3,2-a]pyridine-7-carboxylic acid (CCA) are described in [1].

Absorption, fluorescence and phosphorescence spectra of the aqueous solutions of CCA and TPA were studied. Absorption spectra of these compounds are in the interval $\lambda \leq 450$ nm and have three maxima at 216 nm, 244 nm and 345 nm. Absorption spectra of CCA and TPA differ weakly. The fluorescence spectrum has shown a maximum at about 420 nm. The fluorescence excitation spectrum and absorption spectrum of the compounds are similar thus we can conclude that the molecule has one fluorescence center. According to [2] we estimated the energy of the first electron transition 0-0 and next electron-vibrational transitions for TPA and CCA. Also from the phosphorescence spectra of the molecules we defined the energy of triplet transitions ($T_1 \rightarrow S_0$).

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Dimerization of viologens in liquid crystalline medium

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It was shown that combining lyotropic liquid crystals (LLC) with electrochromic impurities, namely viologens, allows for creating new liquid crystalline materials with regulated optical properties. Structural and electrooptical properties of such materials were thoroughly investigated in series of works and are summarized in [1, 2]. Possible practical applications require understanding of intermolecular processes causing colour modifications of interest.

In the art there is no consensus on the mechanism of dimerization of viologens in liquid matrices under the action of an electric field. Optical spectra of liquid crystal – viologen samples demonstrate that with increase in applied voltage value viologens reversibly reduced in two steps with formation of blue-coloured radical cations and colourless biradicals. Further increase in voltage leads to the formation of red-coloured dimers. The main absorption band shifts to the violet spectral region. These data along with quantum mechanical theory suggest that dimerization of viologen molecules in liquid crystalline medium occurs due to the interaction between viologen molecules, which were fully reduced under the action of applied electric field, and initial non-reduced viologen molecules.

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Influence of Charge Mobility on Absorption and Fluorescence Spectra of Polymethine Dyes Based on 1,3-Indanedione

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Polymethine dyes continue to be used widely in numerous applications due to their unique electronic and spectral properties which form a basis for the design of new effective materials connected with the light conversion and fluorescent markers. Besides, symmetrical and unsymmetrical polymethine molecules remain convenient objects for developing of new theoretical conceptions and quantum-chemical models. This paper presents the results of both quantum-chemical and spectral investigation of the vinylogous series of symmetrical anionic polymethine dyes derivatives 1,3-indanedione **1** as well as their unsymmetrical analogues **2**, presented in Fig. 1.

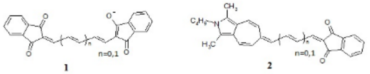

Fig. 1. Chemical formula of studied dyes.

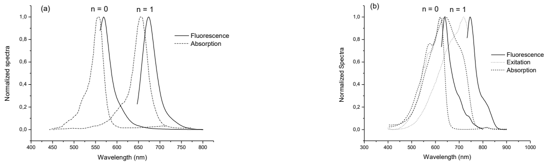

Fig. 2. Normalised absorption, fluorescence and fluorescence excitation spectra of dyes **1** (a) and **2** (b) in acetonitrile.

UV-Vis absorption spectra were recorded on a Shimadzu UV-3100 spectrophotometer in toluene, acetonitrile and ethylene glycol (spectral grade). Fluorescence measurements were performed using fluorescence spectrophotometer Varian Cary Eclipse at low concentrations ($C=10^{-6}$ M) to avoid re-absorption of the fluorescence.

The analysis of the spectral data from Fig. 2 shows the next regularities. Fluorescence spectra demonstrate relatively small Stokes shifts (about 20 nm), that points directly on the comparative slight change in the equilibrium molecular geometry in the excited state upon relaxation to the “fluorescence” or emitted state. Increasing of the length of the chromophore by introducing of the new vinylene group causes increasing of Stokes shifts up to 1,4 times and the regular bathochromic shift (about 100nm) of both band maxima in the absorption and fluorescence spectra.

Structure and IR spectra of triphenyl phosphite

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IR spectra of different phases of triphenyl phosphite (TPP) have been measured in the 400-4000 cm^{-1} spectral range. The strongest differences between the IR spectra of different phases are observed in the spectral regions 1140-1240, 840-900, and 700-800 cm^{-1}. We suggest that conformational mobility of TPP molecule is responsible for these differences.

Computer simulations of the conformers have been performed using the DFT method with B3LYP/6-31 G(d) functional. Geometrical structures of five conformers were obtained during the simulations, which differ from each other in the bond lengths P-O and C-O, and values of the angles O-P-O and P-O-C.

Comparison of the calculated and experimental IR spectra allows us to conclude that in stable and metastable phases are most likely realized conformers, which are close to conformer III. In the glacial, glass and liquid phases are present all five conformers. Phase transitions may be responsible for changes in the conformational mixture. The energies of the conformers in Hartree are equal to -1262,007903 (I), -1262,005736 (II), -1261,991493 (III), -1262,007286 (IV) and -1262,007314 (V).

Significant frequency changes in the IR spectra are observed when going from one conformer to another in C-O and C-C in-plane stretching and benzene ring in-plane bending vibrations in 1140-1240 cm^{-1} region. In the 840-900 cm^{-1} spectral region P-O and C-O in-plane stretching, benzene ring in-plane bending and wagging vibrations manifest themselves. The in-plane stretching and in-plane bending vibrations of PO_3 group and in-plane wagging vibrations of benzene ring manifested themselves in the 700-800 cm^{-1} spectral region.

Namely conformational mobility leads to the formation of broad structureless υ (PO) and υ (CO) bands in the experimental spectra.

Intermolecular hydrogen bonds in solutions of acetic acid. Raman spectra and ab initio calculations

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Bands of C = O vibrations of various aggregated forms in pure acetic acid in the Raman spectra have different values of the depolarization ratio. Ab initio calculations by the Gaussian 98W software in the Hartree-Fock basis set of Gaussian functions RHF 6-31G ++ (d, p) show that this is the way it should be. Thus, the formation of aggregates of molecules leads not only to a change in the dipole moment of the molecules, but also to a change in polarizability tensor of the bond. Calculations based on the mentioned software have shown that one of the hydrogen atoms of the group CH_3 of acetonitrile can participate in intermolecular hydrogen bond. This can lead to the formation of closed dimers acetonitrile-acetic acid. However, comparison of the calculated and experimental data shows that in the case of molecules of acid-acetonitrile the H-bond is formed in the direction of elongation of acetonitrile molecules –O-H…N≡. The activity of one of the hydrogen atoms of the group CH_3 of acetonitrile leads to formation in pure acetonitrile of closed dimeric units with the shift of C≡N band of acetonitrile in the direction of lower frequencies. The low-frequency band asymmetry of C≡N band of acetonitrile in the Raman spectra is associated with the presence of such aggregates in liquid acetonitrile.

Cyclization reaction dynamics of a diarylethene derivative revealed by femtosecond transient absorption spectroscopy

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The transient absorption spectroscopy in combination with ultrashort pulses lasers allows to explore femtosecond dynamics of fast chemical processes. One of the most promising materials for the creation of multifunctional nanodevices, such as heavy metal sensors, organic nano-layers/wires, 3D optical data storages and tumor markers, are the photochromic diarylethene derivatives.

The purpose of this study was to determine the time constant of the photoinduced effect of transition from opened to closed isomer for photochromic diarylethene derivative in ethanol solution by femtosecond "pump-probe". Third harmonic generation (266 nm) of femtosecond Ti:Sapphire laser (Mira-900-F) was used as a pump radiation. As a probe radiation we used supercontinuum generation (450–700 nm), obtained in Al_2O_3 crystal by femtosecond pulses pumping at wavelength 800 nm. Time profile of transient absorption spectrum for photochromic diarylethene molecules presented in Figure 1.

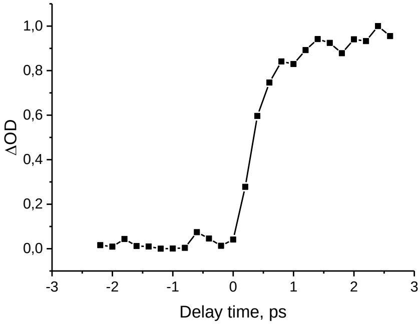

Fig. 1 Time profile of transient absorption for photochromic diarylethene molecules (closed isomer) solved in ethanol solution for the pumping parameters of femtosecond Ti:Saphire laser: λ_{pump} = 266 nm, τ_{pump} = 140 fs.

An analysis of experimental data shows that the time constant of cyclization reaction for photochromic diarylethene derivative is close to 0.9±0.1 ps. The obtained results can be considered as a basis for design of flexible organic electric nanodevices with specified characteristics.

Optical and vibrational spectra of the resveratrol

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Chemical synthesized antitumor drugs have a good bioavailability but high toxic effects to normal tissues. On the other part, the natural drug has unstable properties. It is known that the nanostructure modification of drugs can reduce cytotoxic effects. In the recent years, oxyresveratrol has attracted considerable interest for its beneficial effects for human health: cardiovascular protective effects, anti-inflammatory properties, platelet anti-aggregate and antitumor activity. However, the utilization of beneficial effects of the oxyresveratrol is limited. This molecule is an easily oxidizable and extremely photosensitive.

The geometry of stilbene was optimized. The energy of the ground state and the dipole moments was calculated for these molecules using density functional theory with a hybrid 3 parametric of Becke exchange-correlation functional and functional of Lee-Young-Parr (B3LYP/6-31G (d, p)). The IR and UV spectra of the oxyresveratrol were computed. The energy of solvation of the oxyresveratrol was defined. The IR spectra of the oxyresveratrol in the various solvents were measured. The solvent influence on the optical parameters and bioactivity of the oxyresveratrol was shown.

The possibility of formation charge-transfer complexes and the existence of molecular interaction had been proved using small angles neutron scattering, Surface-enhanced Raman scattering spectroscopy, infrared absorption spectroscopy and UV spectroscopy.

The emission lifetimes of the Eu(III) and La(III)-Eu(III) doped complexes based on cardacylamidophosphate ligand

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Effective sensitization of the lanthanide emission was expected for the coordination compounds with 2,2,2-trichloro-N-(dipiperidin-1-yl-phosphoryl)acetamide (HPip), $Cl_3CC(O)N(H)P(O)[N(CH_2)_5]_2$ which contain the additional “antenna ligand” - 1,10-Phenantroline. Luminescence decay curves were recorded for complexes $[Eu(Pip)_3(Phen)]$ and $[La_xEu_{1-x}(Pip)_3(Phen)]$ (x = 0.99, 0.95, 0.50) using microsecond time-correlated single photon counting option of FLS920 setup (Edinburgh instruments Ltd).

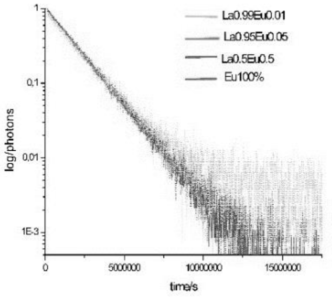

Fig. 1. The luminescence decay curves recorded at 77 K

Decay time of the $[Eu(Pip)_3(Phen)]$ emission is temperature independent, and thus reflects the absence of thermally activated nonradiative processes, either vibrational or electronic in nature, including the $^5D_0$ state. With decreasing of the Eu^{3+} concentration the emission decay time extends what can be explained by the temperature dependent energy migration process observed for all doped compounds. Moreover, for $[La_{1-x}Eu_x(Pip)_3(Phen)]$ (x = 0.05 and x = 0.01) at 77 K the second component of the decay time of the order of 20 ms appears.

This is related to the ligand phosphorescence due to the high $[La(Pip)_3(Phen)]$ concentration. To confirm this the emission decay times for all europium complexes at 77 K were measured exciting the $^5D_2$ level of the Eu^{3+} ion (λ_{exc} = 464.5 nm). It is found that the curves keep an exponential decay without long-lived component (τ=1.61 ms for Eu 100%, 1.69 ms for Eu 5o%, 1.68 ms for Eu 5% and 1.71 ms for Eu 1%.

Charge Mobility and Localization of the Second Higher Excited State in Merocyanine Dyes, Using Spectral Methods

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This paper presents the results of quantum-chemical calculation and spectral investigation of merocyanine dyes 1-butyl-2-methylquinolinium p-toluenesulfonate with two chain lengths. Their formulae are presented in fig. 1.

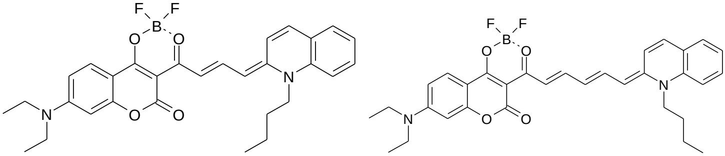

Fig. 1. Chemical formulas of investigated dyes.

The aim is to study the spectral properties of a meroccyanine dyes, depending on the chemical structure, in particular, their chain length, the study of transitions to higher excited states, especially in the second higher excited state. For this we carried out experimental spectral measurements of dyes and the corresponding numerical calculations.

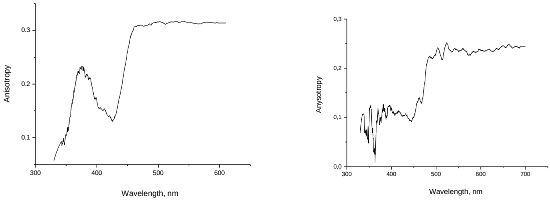

Figure 2. Anysotropy spectra of investigated dyes.

Anisotropy spectra were recorded on a Cary Eclipse Fluorescence Spectrophotometer in ethylene glycol. Quantum-chemical calculation of optimized molecular geometry were performed DFT/CAM-B3LYP//6-31(d,p) method; the electron transition characteristics were calculated by the non-empirical (TD/DFT/6-31G(d,p)/CAM-B3LYP) method, using the package Gauss-03.

It was shown experimental and theoretical localization of second higher excited state.

Temperature evolution of cluster structure in n-hexanol, isolated in Ar and N_2 matrices and in condensed states

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This work is devoted to the investigations of alcohol clusters. Monohydric alcohols are used as model objects, because their basic hydrogen bond topology is simple and may serve as an elementary starting point for the investigations of complex three-dimensional hydrogen-bonded networks. Monohydric alcohols contain only one hydroxyl group that simplifies calculations and the assignment of the spectral bands. Using FTIR spectroscopy we observed the temperature evolution of the cluster structure of n-hexanol, isolated in argon and N_2 matrices, and in condensed states. Quantum chemical calculations are used for the interpretation of the registered FTIR spectra and for the assignment the bands within the limits of the method precision.

The spectra of photoluminescence and luminescence under X – ray excitation have a different form

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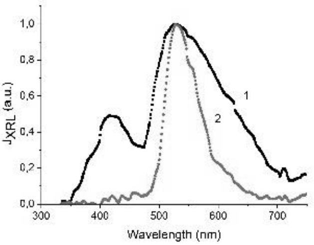
Experiments was performed using 3 – Hydroxyflavone (3HF) in toluene solution in range of concentrations from 0.0625 $^{g}/_{L}$ ($1.566 \cdot 10^{17}$ cm^{-3}) to 64 $^{g}/_{L}$ ($1.6 \cdot 10^{20}$ cm^{-3}). The sample 3HF was chosen because it has a high Stokes shift of fluorescence band, which allows to avoid the effect of self – absorption of PL in a sample [1].

Each experimental sample for luminescence under X – ray excitation (XRL) researches was irradiated by X – ray tube БХВ – Re (20 kV, 25 mA) and for photoluminescence (PL) was excited by nitrogen laser (337 nm, 29700 cm^{-1}). Light from sample was detected in visible region by the FEU – 106 photomultiplier. Spectral measurements were carried out using a monochromator MDR – 2.

The typical spectra of PL (1) and XRL (2) at room temperature for 3HF in toluene for concentration 1 $^{g}/_{L}$ are shown below.



There is a fundamental difference in the mechanism of PL and XRL excitation. In former case occurs the absorption of excitation quantum by photochromic molecule itself (one absorbed quantum leads to one excitation), while in latter excitation quanta are absorbed by molecules of the solvent, which will lead to generation of high – energy electron. During thermalization of such an electron in small volume of the matter hundreds – thousands of electronic excitation are produced. After occurring migrations over molecules of the solvent, electronic excitations can relax without any irradiations or transfer their excitation energy to photochromic molecules. In the second case we deal with relaxation of excitation on photochromic molecule which occurs alongside irradiation of the luminescent quantum [2, 3].

[1] Wu Feng, Lin Lie, Li Xiang - Ping, Yu Ya - Xin, Zhang Gui - Lan, Chen Wen - Ju, All – optical switching of 3 – Hydroxyfavone in different solvents, Chin. Phys. B, Vol. 17 № 4 (2008), 1674-1056.

[2] V. M. Agranovich, M. D. Galanin, Electron excitation energy transfer in condensed matter, Nayka, Moscow, 1978, pp. 300 – 384 [in Russian].

[3] A. A. Ishchenko, Structure and spectral – luminescent properties of polymethine dyes, Naukova dumka, Kyiv, 1994 [in Russian].

Experimental study of thermodynamics properties of magnetic liquid system stabilized by single layer of lemon acid

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Magnetic liquid system has a unique combination of fluidity and the ability to interact with magnetic field. Properties of ferrofluid are defined as the set of characteristics of components that it contains. The properties are possible to change in wide limits that can changes the suspension settings [1].

The interest in studying magnetic liquid systems is related to unusual combination of properties of magnetic materials, liquids and colloidal solutes. Magnetic fluids can be applied in various fields of technology (to create ferrofluidic seals in chemical industry, magnetic oils and different cooling systems, suspension brackets with regulated stiffness in automotive industry) as well as in biology and medicine [2].

Thermodynamic properties of magnetic fluid system stabilized by single layer of lemon acid are investigated. The aim of work to conduct $P-V-T$ measurements of magnetic liquid system based on water, stabilized by lemon aced in the pressure range from $0.1\ MPa$ to $101\ MPa$ and the temperature from $303\ K$ to $345\ K$. The coefficient of thermal expansion α_p, modulus of elasticity K_T, isothermal growth of Gibbs potential ΔG, isothermal increase of entropy $T\Delta S$ and internal energy ΔU was found.

The experiment shows that adding of magnetic substance in water leads to significant increase in modulus of elasticity K_T and the corresponding change in growth of internal energy ΔU. The results of experiment are compared with the results obtained for water.

[1] Bulavin L.A., Moroz K.O., Nedyak S.P., Petrenko V.I. The Equation of State for a Water-Based Magnetic Fluid Stabilized by Lauric Acid / Ukr. J. Phys. 2012, Vol. 57, N 3, p.350-354.

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X-ray study of substituted tert-butyl-calix[4]arenes

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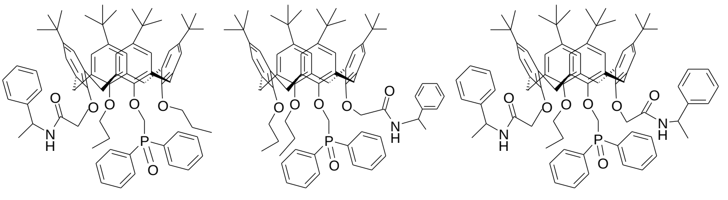
Calixarenes – a phenolic macrocyclic compounds having intramolecular cup-like cavity formed by aromatic fragments macrocyclic skeleton, connected through a methylene group. Calixarenes, thanks to its unique shape, occupy an important place in supramolecular chemistry [1]. They exhibit the ability to recognize and bind to stable complexes, and share similar properties cations, anions and neutral molecules.

We have investigated the next calixarenes [2] (Fig. 1):

1) 5,11,17,23-tetra-tert-butyl-25,26-methoxy-propane-27-(1`-phenyl-enthylamino)-methoxypropane-28-methoxy-methylphosphinoyl-methane-(1`-diphenyl)-calix[4]arene ($C_{73}H_{90}NO_6P_1$);
2) 5,11,17,23-tetra-tert-butyl-25-(1`-phenyl-enthylamino)-methoxypropane-26,27-methoxy-propane-28-methoxy-methylphosphinoyl-methane-(1`-diphenyl)-calix[4]arene ($C_{73}H_{90}NO_6P_1$);
3) 5,11,17,23-tetra-tert-butyl-25-methoxypropane-26,27-(1`-phenyl-enthylamino)-methoxypropane-28-methoxy-N(1'-phenyl-ethyl)-acetam-calix[4]arene ($C_{80}H_{94}N_2O_7P_1$).



1) 2) 3)

Fig.1. Structural formulas of the studied calix[4]arenes.

The single crystal x-ray diffraction study was performed for determination of the molecular and crystal structure of substance. It was found that these compounds in solid state adopt cone conformation. Usually these compounds make supramolecular complex with solvent from which crystals were grown. The guest molecules could be placed inside of calixarene cavity as well as outside.

These compounds are very promising for creating new extractants for radioactive waste, supramolecular catalysts chemo- and biosensors [3].

[1] J.W. Steed and J.L. Atwood, Supramolecular chemistry, 2nd Ed. (New-York, 2000), pp. 22-24.
[2] V.I. Boyko, O.A. Esipenko et. all, Tetrahedron Lett., in press.
[3] C.D. Gutsche, Calixarenes: An Introduction, (The Royal Society of Chemistry: Cambridge, 2008), pp. 18-20.

Polymorph modifications of $C_{18}H_{17}F_3N_2O_4S$

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As a result of X-ray investigation recently synthesized $C_{18}H_{17}F_3N_2O_4S$ (Fig.1) (new precursor for biologically active compounds) was found that this compound under identical conditions crystallized in the three polymorphic modifications.

The main difference is the type of intermolecular H-bonds pattern (Fig.2). The molecules of **α** by the quite strong intermolecular H-bonds are connected in centrosymmetric dimers which in turn are organized in 2D chains-net. The molecules of **β** by the system of the fork H-bonds form dimers, which are organized in 1D zig-zag chains. The molecules of **γ** by type H-bond similar to the molecules of **α**, they by the quite strong intermolecular H-bonds are connected in centrosymmetric dimmers which in turn are organized in 2D net.

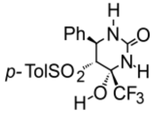
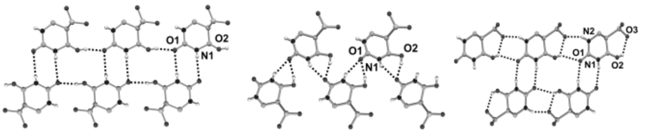


Fig.1 The structural formula of



α **β** **γ**

Fig. 2. Intermolecular H-bonds in **α**, **β** and **γ** polymorphs.

The molecules of **α** and **β** polymorphs has very similar molecular geometry, except the slight difference of the core heterocycle N(1)N(2)C(1-4) conformation: for **α** – flattened half chair; for **β** – flattened half bath; for **γ** – flattened half bath.

In the Raman spectrum of this compound (Fig.3) observed number of lines that can be attributed to the vibrational modes of structural fragments of molecules. For example, benzene fragment comprising atoms C(6)-C(11), the spectral lines correspond to 996 cm^{-1}, 608 and 850 cm^{-1}. The lines 626, 728, 1005, 1031, 1207, 1212 cm^{-1} in the Raman spectrum belong to fluctuations in toluene.

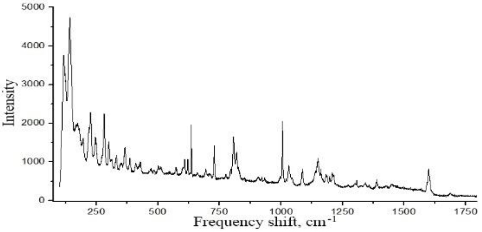


Fig. 3 Raman spectra for a mixture of **α**, **β** and **γ** polymorphs of compound $C_{18}H_{17}F_3N_2O_4S$.

Formation of Textures in the Dried Na-DNA films at Different Concentration of DNA in the System

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The research deals with the films of Na-DNA water solution dried at temperature 20°C and 42°C. With the help of a microscope with the special ocular lens connected to the camera there have been received the pictures of films with various concentration of DNA (from 0.1 to 1%, with a step of 0.02%). For analyzing the structural peculiarities of the films a special computer program has been developed. Upon the results of the computations a ratio of the texture area to the film area has been obtained for every picture. The DNA has been established to induce formation of textures on the film surface. The dried films without DNA do not have the textures. As DNA concentration increases the texture area grows. The textures differ at the different temperatures. At the higher temperature they are denser.

FTIR spectra of n-pentanol and n-octanol in liquid and solid state

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Alcohol molecules can form hydrogen bonds and arrange in different structures named clusters. The aim of this work is to study the behavior of cluster structure of alcohols at phase transitions and to research the structure of investigated alcohols in solid and liquid state.

Objects of investigation are monohydric alcohols n-pentanol $(CH_2)_4CH_3$–OH and n-octanol $(CH_2)_7CH_3$–OH. Matrix isolation FTIR spectroscopy was used for investigating individual alcohol clusters. FTIR spectra of n-pentanol and n-octanol in condensed state were registered. Special attention is paid to the investigation of the behavior of different clusters at the phase transition temperature. In order to interpret the experimental spectra quantum – chemical calculations using Gaussian 03 software (approximation DFT/B3LYP, 6 – 31G (d, p) was used.

Spectroscopic study of luminescent centres in solutions with copper complexes

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The present work is devoted to a consideration of the spectral properties of haloid and phosphorus-containing concentrated solutions activated with copper complexes (10^{-3} – 10^{-1} mol/l).

The solutions with a copper ion impurity were investigated by the absorption, photoluminescence (PL), PL excitation methods in the temperature range of 4.2 – 300 K.

The observed spectra are conditioned by the electron transitions between the energy levels of the Cu^+ ion which are deformed due to the interaction with an environment.

Reducing the temperature of studied solutions down to 4.2 K results in a considerable shift of PL peaks towards a short wavelength region.

The luminescence quantum yield of the solutions with copper complexes was analyzed in the temperature range of 77 – 160 K. It is found that the temperature-dependent shifts of PL bands of studied solution are closely bound with the quantum yield of luminescence.

It is shown that the activation energies (Q) of nonradiative transitions in the solutions concerned are substantially lower than those in phosphors of the same composition.

Influence of electromagnetic radiation on energy self-consistent field structure of liquids

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Linewidths ($\Delta\nu_{1/2}$, cm^{-1}) of the depolarized component ($I_{\perp}$) of Rayleigh scattering light (RLS) in benzene (C_6H_6), methyl iodide (CH_3I) and chloroform (CH_3I) versus frequency (λ, Å) and intensity ($I_{otn.}$) of exciting radiation were investigated. Tables 1 and 2 show the results of the study ablation.

Table 1.

λ, Å	C_6H_6	CH_3I	$CHCI_3$
4765	4,8	2,3	2,9
4880	4,8	2,2	2,74
4965	4,6	2,1	2,5
6328	3,4	1,7	1,6

Table 2.

I_{rel}	10	50	100	500	2000	5000	10000
$\Delta\nu_{1/2}$	5,3	5,3	5,1	5,1	4,86	4,3	4,3

As a result of the vibrating influence of the physical vacuum [1] and the surrounding molecules a particle wave function of response (WFR) is formed [2]. As a result of the phase correlation between the WFR molecules self-consistent field fluids are formed. Energy structure of the depolarized component of RLS can be represented as a superposition of the cores and the WFR Brownian molecules. Central component in the circuit PPC is due to the concentration and energy structure of WEF Brownian molecules [3].

As a result, the influence of an exciting radiation leads to the change of the energy structure of the self-consistent field fluids. In discussing of the results in Table 1 the ratio between the spatial resolution WEF Brownian molecules on the wavelength should be taken into account. You may notice that long-wave radiation has the ordering influence and reduces the concentration of Brownian molecules and, consequently, causes a narrowing of the line widths of the PPC. Increase the intensity of the exciting radiation is accompanied by ordering in the self-consistent field fluids and increasing the phase coherence between the WEF molecules. Reducing of the concentration of Brownian molecules occurs that leads to narrowing of the wing of light scattering line (Table 2).

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Field-substance interaction and energetic structure of molecular liquids

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Eddy processes of self-organization and self-compression in the physical vacuum affct all real particles and bodies. They can be regarded as an area of thickening of the physical vacuum or vacuum fluid. Moreover, the physical vacuum energy density is much higher than the energy density of an atomic nucleus [1].

The energy structure of substances depends on the nature of the interaction of individual units of material to a vacuum and the surrounding fluid particles. Depending on the frequency of oscillation of a material unit formed wave function of response (WFR) particles [2], which has the properties of the respiratory vibration. Molecular substance can be represented as a hierarchy of units of material having natural frequencies. Phase correlation between WFR related materiel units will result in a hierarchy of nested and self-consistent fields or imposed hierarchy energy structure of the medium.

1. The interaction between field-matter and the outer electrons of the surrounding molecules form WFR combined electrons. Energy structure of WFR combined electrons manifests as broadband background in Raman spectra [2].

2. Phase correlation between WFR center of gravity of the molecules will self-consistent field WEF formation of a molecule or the formation of an acoustic field environment. It manifests itself in the form of Mandelshtam-Brillouin light scattering.

3. As a result, the phase correlation between the WEF cores molecules forms self-consistent field WFR cores molecules. It manifests itself in the form of high-frequency wing of the neutron spectrum and the Rayleigh scattering of light [2].

4. Atomic frequency vibrations are significantly different from the oscillation frequency of the core molecules as a whole. Energy structure of WFR cores of molecules is projected on the energy structure of the WEF atomic vibrations. This leads to the formation of side branches of the S and O in the spectrum of Raman scattering of light, the side branches of P- and R- in the infrared absorption spectrum.

5. The frequency of oscillation or vibration WEF supramolecular structures is much smaller than the oscillation frequency of the molecules as a whole. They are manifested in the form of low-frequency component in the spectrum of the neutron and the Rayleigh scattering of light [2].

6. Violation of the phase correlation of individual particles with the environment leads to the appearance of Brownian particles, depending on the energy structure of the WFR Brownian molecules form a central component in the spectrum of the Rayleigh scattering of light.

[1] Chernin A. D. Cosmic vacuum, Physics Uspekhi, v.171, p.1153 (2001).

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Demonstration of “memory” effect at the phase transition liquid-crystal

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“Various parameters (peak intensity, frequency, width) of IR absorption bands of a number of substances in the vicinity of the phase transition liquid - crystal (PhTLR) were investigated in a cycle of heating and cooling. In the heating cycle a temperature stabilization of the analyte in a certain temperature was carried out, after which the parameters of IR absorption bands were recorded. In the refrigeration cycle a speed of temperature reduction was different, and IR spectra were registered continuously.

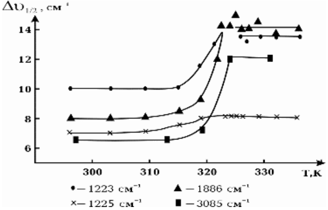

Fig. 1. The dependence of IR bandwidth of diphenyl on temperature in heating cycle in the vicinity of a phase transition liquid-crystal.

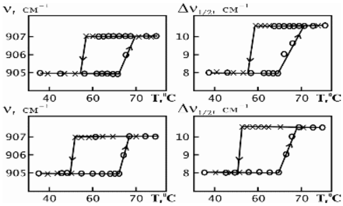

Fig. 2. Change of frequency (ν) and width ($\Delta\nu_{1/2}$) of diphenyl at phase transition liquid-crystal in cycle heating-cooling at cooling rates of 0.4 (a) and 2 grad/min (b).

When approaching the phase transition point of the crystal in the liquid phase in a narrow temperature range there is a relatively rapid increase in the width of the absorption band, and in the liquid state this change is exponential (Fig.1).

During sample cooling a hysteresis was observed in the behavior of various parameters of the IR absorption bands. The width of the hysteresis loop depends on the cooling rate of the substance. Hysteresis is observed in the behavior of the magnitude of the peak intensity. There is an abrupt decrease in its value at the phase transition of a substance from a liquid state to a crystalline phase. There is an abrupt decrease or increase of the value of the absorption band frequencies depending on the symmetry of vibrations.

Results of the study explaine the behavior of the energy structure of the self-consistent field agents [1] and an abrupt change in the concentration of molecules in Brownian phase transition liquid-crystal. Hysteresis is associated with structural "memory" of the substance, the recovery of which depends on the concentration and rate of absorption of Brownian molecules.”

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Temperature dependence parameters of the lines Raman light scattering in dioxane

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The problem of establishing of the nature and power of intermolecular interactions (II) in condensed matter, as well as the most common patterns of change in the optical spectra of complex molecules, a phenomenon due to the different nature of the II is a fundamental area of modern condensed matter spectroscopy.

Our task was to study the temperature dependence of some parameters of the spectrum of Raman light scattering (RLS) - half-width, intensity, shape, contour, etc. The object of investigation was dioxane ($C_4H_8O_2$) - a dipole-free, axially symmetric polarizability of the molecule.

Raman spectra were recorded using the experimental setup, collected on the basis of a DFS-12 spectrometer, which is designed to produce a faint glow in the automatic mode [1]. The Raman spectra were studied in the temperature range from 20 to 150^{o}C.

The results of experimental studies of RLS show that throughout the investigated temperature range there is a general upward trend in half-width. However, the rate of change of the half-width varies with temperature in various temperature ranges. Anomalous behavior of the half-width in the temperature 65-80^{o}C we associate with changes in short-range order in the liquid. The integrated intensity of all the lines tends to fall with increasing temperature.

It is worth to note the fact that in the temperature 65-80 ^{o}C there are anomalies both in the integrated intensity and in the half-width. The intensity of all the lines of cattle in 65-80 ^{o}C experiences a slight rise, and then drops again with a further rise in temperature. We attribute the change to the integrated intensity of the change in the correlation factor γ [2].

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Refractometry of water-ethanol solutions near the peculiarity of the contraction

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The work is devoted to the experimental study of the refractive index`s concentration dependence in equilibrium water-ethanol solutions. Particular attention is paid to the solutions` behavior in the vicinity of a peculiar point defined as the point of intersection of the contractions at different temperatures or the point at which there is a maximum intensity of the molecular light scattering. It is found that the refractive index noticeably deviates from its reference values in the vicinity of the peculiar point $0.05 < x < 0.1$ (x-mole fraction of ethanol). This effect reflects the fact that the equilibrium properties of the solutions are established only in a few weeks.

The arguments to prove that in this concentration range the system becomes micro inhomogeneous are presented. Devoted to the study of irreducible two-particle factors to the refractive properties of liquids and solutions. The two-particle factor to the polarization vector of the system is measured by electrostatic methods due to small deformations and overlaps of the atomic and molecular shells. It is established that the molecular refractive index of binary solutions became a weakly non-additive function of the refractive indexes of its components when the two-particle factor is taken into account. At the example of aqueous ethanol and methanol solutions, it is shown that the obtained refractive indexes of solutions precisely agree with the experimental data.

Specific and universal intermolecular interactions in solutions of some zwitterionic compounds

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Zwitterionic compounds have the opposite charges separated on two adjacent atoms and posses great dipole moments in their ground states. The visible photons can induce charge transfer transitions, with small spectral intensities and very sensitive to the solvent nature. Depending on the charge transfer directions, the molecular dipole moments in the excited states of this type of compounds can be smaller, or higher than those in the ground states of the zwitterionic molecules. The spectral bands due to the charge transfer are shifted to blue, respectively to red in function of the values of the dipole moments in the excited states of zwitterionic compounds. The spectral shifts in solvents with different nature offer information about the changes in dipolar nature of the zwitterionic compounds.

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8

Nanoobjects

NMR and FTIR spectroscopy study of materials for innovative medicine: sol-gel derived calcium hydroxyapatites

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Hydroxyapatites are widely applied in implantology, orthopedic and periodontal surgery [1]. Calcium hydroxyapatite ($Ca_{10}(PO_4)_6(OH)_2$, further CaHA) has been often used to study the properties of antiresorptive agents for the prevention and treatment of bone diseases.

CaHA containing amorphous phosphate phase (ACP-CaHA) and nano-structured one have been prepared by two sol-gel synthesis routes. The structural organization of hydroxyl groups in both materials has been determined by means of ^{1}H MAS NMR and FTIR spectroscopy. It has been shown that the amount of structural –OH groups in nano-structured CaHA is significantly higher than that from adsorbed water and *vice-verse* in ACP-CaHA. A precise signal shape analysis has been carried out for both studied samples [2]. The ^{31}P NMR signals have been found being Voigt-shaped as in the static as well as in MAS spectra. The spin-lattice and spin-spin relaxation times measurements have revealed the fast spin motion takes place in ACP-CaHA. The corresponding correlation time $\tau \sim 7\cdot10^{-7}$ s at 300 K has been determined. The dynamics of ^{1}H–^{31}P spin interactions in nano-structured CaHA ($\tau \sim 3.3\cdot10^{-5}$ s) is much slower than in ACP-CaHA.

The magnitude of the anisotropic broadening 1220 ± 20 Hz determined for nano-structured CaHA is very close to the maximum of the dipolar ^{1}H–^{31}P coupling distribution profile estimated using CP MAS kinetics.

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Spectroscopy of the Sm^{3+} ions in the $LaVO_4$ compositions

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Investigated the $La_{1-x}Sm_xVO_4$ powder sample series are presented by compositions with x = 0.05 ÷ 0.4 and synthesized by both co-precipitation and sol-gel methods. Phase compositions and crystal lattice parameters were determined by XRD spectroscopy. The $LaVO_4$ samples possess monoclinic structure, whereas the $La_{1-x}Sm_xVO_4$ compositions transform in tetragonal structure at $x > 0.1$. The microstructure of the obtained compounds was studied with SEM. Average grain sizes of powders synthesized by co-precipitation method is in several times smaller than average grain sizes of powders synthesized by sol-gel method. Besides, sol-gel particles have tendency to create conglomerates, whereas solid state synthesis and co-precipitation posses free grain nanopowders.

Luminescence spectra contain spectral lines in 550 – 570, 580 – 620, 630 – 660, and 690 – 720 spectral ranges. These spectral lines are caused by inner *f-f* electron transitions in the impurity Sm^{3+} ions. Number of spectral lines, their relative distributions and intensities depend on method of synthesis. We suppose that two types of the Sm^{3+} centers can be formed in the vanadate matrix.

Two types of centers have been observed previously for the $La_{1-x}Eu_xVO_4$ compositions only at low Eu^{3+} concentrations and were supposed to be formed by residual inclusions of monoclinic phase in tetragonal crystal lattice or Eu^{3+} ions on grain's surfaces. For the investigated heavy doped nanoparticles only the latter explanation is possible. Structure of the both types of Sm^{3+} luminescence centers is discussed.

Dye adsorption from aqueous solution by mesoporous calcium carbonate microparticles $CaCO_3$

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Currently, the use of micro - and nano-scale materials, including nanoparticles and mesoporous materials of different chemical composition as a platform for encapsulation or adsorption diagnostics, drugs and other active agents for their interstitial / intracellular delivery is relevant and promising scientific task, the successful solution of which is associated with a breakthrough in the treatment of many diseases.

This work is devoted to the synthesis of microspheres of calcium carbonate $CaCO_3$ with polymorph modification vaterite, characterization and studying their adsorption capacity. As a model system of loaded organic molecules, we used Rhodamine 6G (R6G) and Methylene blue (MB) dyes, that made it possible to study the mechanisms and adsorption kinetics by optical spectroscopy methods.

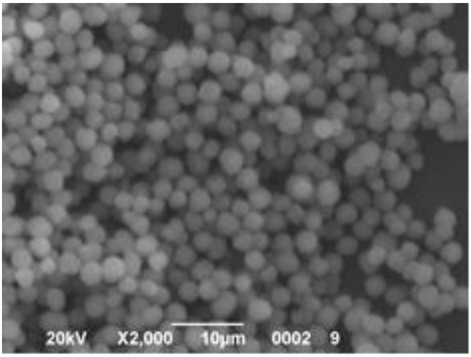

Fig.1. SEM image of synthesized $CaCO_3$ microparticles.

Using structure-directing agent poly(sodium 4-styrenesulfonate) PSS allow us to synthesize mesoporous $CaCO_3$ microparticles of 3 μm average diameter with prevalent polymorph vaterite. It has been shown that adsorption process for both dyes were well fitted by Freundlich isotherm and pseudo-first order kinetic. The adsorption capacity of $CaCO_3$ microparticles is found to increases 10 times as compared to CaCO3 microparticles synthesized without PSS. The adsorption process is diffusion-mixed, i.e. is controlled by diffusion of dye in the film solution and diffusion in the pores of the adsorbent depending on the contact time of the adsorbent and adsorbate.

Raman and X-ray diagnostics of nanocrystals grown from the $Bi_{12}SiO_{20}$ melt in synthetic opal pores

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$Bi_{12}SiO_{20}$ is a very famous material with prominent physical properties. The obtaining and investigation of its nanocrystals in opal pores is interested in physics of low-dimensional systems and applied physics.

Polycrystalline $Bi_{12}SiO_{20}$ powder placed on the opal surface was slowly heated up to 900 ^{0}C (higher than the melting temperature) and then cooled to room temperature at the same rate. The most part of melt entered the opal due to capillary effect. The structure analysis of the samples was made by Raman spectroscopy and X-ray diffraction (XRD) methods.

Both methods proved crystalline state of the embedded substance. The XRD pattern is rather similar to the γ-Bi_2O_3 pattern than to the $Bi_{12}SiO_{20}$ powder one. In Raman spectrum (compared with the $Bi_{12}SiO_{20}$ powder one) new bands appear and some bands, assigned to SiO_4 internal vibrations, vanish within a 250 – 600 cm^{-1} range. The most of low-frequency bands is shifted in accompany with spectral intensity re-distribution.

The results may be explained by assuming structural and chemical composition changes in the nanocrystals. According to [1], when Si^{4+} ion is leaving its place in tetrahedron together with neighbouring oxygen atom (their deposition on the SiO_2 globule surface is not excluded); the γ-Bi_2O_3 structure is formed by partial filling the cation vacancies with Bi^{3+} ions. The Bi-O distances in this umbrella-like group are correlated with the spectral range, where new bands appear [2].

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Structure and vibrational spectra of magic CdSe nanoclusters

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Among different kinds of nanostructures ultra-stable, so-called “magic”, nanoclusters posse special position. Their elevated stability comes from peculiar structure substantially different both from bulk crystal and small molecules. Carbon fullerenes are probably the best known example but not the most unusual. Actually, their structure is determined by the properties of sp^2 hybridized atomic bonds and not by special size-dependent properties. Another example of specific structure of nanoclusters is icosahedral symmetry of atomic arrangement in small noble metal particles. This structure provides packing density higher than FCC or HCP and hence elevated stability and other interesting physical properties. It should be brought into attention that determination of the structure of nanoclusters is not easy task. Lack of translational symmetry of crystals makes X-ray diffraction methods inefficient, signals are weak and diffraction patterns are not sharp. Thus, in most cases the structure of non-crystalline nanoclusters is a result of theoretical prediction based on the first principle calculations.

In present report we consider such structure predictions for magic CdSe nanoclusters, namely $(CdSe)_{13}$, $(CdSe)_{33}$, $(CdSe)_{34}$, and $(CdSe)_{48}$. There most stable suggested structure can be described as nested cages, which are based on closed shells with additional bonding between them. Also we discuss possible methods of experimental verification of these structures. Raman spectra can be suggested since they are very structure-sensitive and easy to realize with the minimal amount of substance. In some cases surface enhanced Raman spectra (SERS) can be measured from single molecules. Results of calculation of Raman spectra for magic CdSe nanoclusters and their comparison with experimental ones are under discussion.

Photoelectrical properties of ITO-pSi structures

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The silicon barrier structures modified with Indium tin oxide (ITO) layer have been widely studied over the last decade because of its photovoltaic properties and possibilities to improve the performance of the solar cells. ITO is one of the most widely used transparent conducting oxides due to its two chief properties, electrical conductivity and optical transparency.

The current-voltage (*I*-*V*) curves and spectral dependences of photovoltage were studied for ITO-*p*Si structures with different thickness of ITO layer (12-100 nm). The ITO layers were found to induce Schottky – type potential barrier causing an observation of nonlinear *I*-*V* curves and photosensitivity of the studied sample in the spectral range from 1.0 eV to 3.0 eV. We have found that increasing of ITO layer thickness causes the increase of potential barrier, which rectify current. As a results, the inner quantum efficiency exhibits growth due to spatial separation of electron-hole pairs by potential barrier.

Nonlinear self-dispersion liquids in critical region

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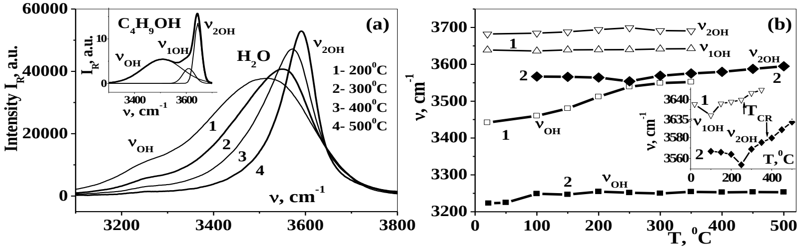
The purpose of this report is development of modern ideas about properties of liquids in critical region. In conditions of strong thermal excitation of vibrations, the role of nonlinear interaction (NI) of vibrational modes with an excitation of higher vibrational states strengthens. This leads to a strong vibration-electron coupling (VEC) and strengthening of interparticle interactions. VEC leads to instability of continuous structure of liquid and its self-dispersion. This weakens the spatial accumulation of NI vibrations and through self-compression by clots (globules) of liquid ensures the existence condensed phase far in supercritical region.

New nonlinear-quantum regularity can be demonstrated on basis of vibrational spectra of water and butanol in critical and supercritical regions ($T \geq T_{CR}$, $P > P_{CR}$) [1, 2]. Fig.1 shows the change in a shape of stretching band of water ν_{OH} in Raman spectrum at T=200-500^{0}C (T_{CR}=374^{0}C) and a pressure of $P=10^3$ bar> P_{CR}=221 bar. In spectra of H_2O and C_4H_9OH in OH band there are always three spectral components ν_{OH} and $\nu_{1,2OH}$. For butanol at T=200^{0}C~T_{CR} and P=500 bar>P_{CR}=41 bar they are shown in inset of Fig.1a. Low-frequency band $\boldsymbol{\nu}_{OH} \approx 3250$ cm^{-1} for water and $\boldsymbol{\nu}_{OH} \approx 3450$ cm^{-1} for butanol belong to liquid phase, which is stored away in supercritical region. Increase these frequencies at P=const and increasing T shown in Fig.1b and is associated with self-compression of liquids in nanoglobules ~ 20 ÷ 200 nm. High-frequency line $\boldsymbol{\nu}_{1,2OH} > \boldsymbol{\nu}_{OH}$ in about 3600 cm^{-1} arises long before T_{CR} and changes with increasing T. According to quantum-chemical calculations the lines $\boldsymbol{\nu}_{1,2OH}$ refer to molecular clusters. The frequencies $\boldsymbol{\nu}_{1OH} < \boldsymbol{\nu}_{2OH}$ belong to bound OH groups, and $\boldsymbol{\nu}_{2OH}$ - to free groups. Changing frequency $\boldsymbol{\nu}_{1,2OH}$ of water and butanol is shown in inset of Fig.1b. Increase of frequency $\boldsymbol{\nu}_{1,2OH}$ at $T > T_{CR}$ is undoubtedly due to the nonlinear self-compression. Because of VEC and changes of chemical bonds liquids in CR have unique properties.



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Conformation effects and photoluminescence spectra of nanocomposition liquid crystals 5CB-carbon nanotubes

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Liquid crystals (LC) are widely used in modern electronic and optical devices. By adding in LC a few nanoparticles of different nature, form, size and surface's condition it is possible to change characteristic of resulted nanocomposite.

The aim of this work is to identify the reasons and mechanism in experimental observed changes of spectral-luminescent properties nanocomposite LC 5CB – CNT (carbon nanotubes) in wide temperature interval.

It is found that in case of temperature rising from 4.2 up to 300 K fluorescence's shift spectrum both pure 5CB and nanocomposite 5CB – CNT on 27.2 and 10.7 nm respectively takes place. Mentioned displacements moving 5CB from solid-state to liquid crystal nematic phase are caused primarily by forming dimeric structure of molecules 5CB and implementing more planar conformation molecules, which first electron level energy is lower, then in twist conformer.

It is shown, that within interval 220 – 260 K sharply drastic changes of maxima of the bands and their half-widths pure and doped luminescence spectra's appears. The amplitude of this changes for composites is 3 times lower than for pure LC 5CB.

Correlation between luminescent properties of the composites 5 CB-CNT, its thermodynamic characteristics received with Differential Scanning Calorimetry method was revealed. The set of all experimental results shows that all observed changes in pure and doped luminescence spectra's LC 5CB are due to phases transformation of crystals and conformational change of the molecule 5CB.

The work was funded by NAS of Ukraine projects VC-157 and V-153.

If there are any opportunities to use carbon micro/nano sized particles as optical materials?

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Carbon micro/nano sized materials (CMNM) are well known and they are regarded as perspective for various applications. At the same time, it should be noted an attention is usually paid to nanoelectronic's usage and not to optical perspectives. There are a set of papers where the PL emissions in CMNM was observed and it has been assigned to various origins. At the same time, lack of data about optical properties of various CMNM is evident; especially it concerns photoluminescence (PL).

This work clarifies the up to now view of CMNM optical properties and their state-of-art applications. Own made experimental and calculation finding are presented too. Today various types of CMNM preparation (graphene is among them) are known. In spite that, development of new methods for fabrication of graphene – like structured materials is still under investigation. We used modified electro-chemical dispersion, called by us as electro-chemical exfoliation method, to prepare graphene containing colloid carbon material. Luminescence, Raman spectroscopy, optical absorption, AFM, ATM, SEM and optical luminescent microscopy (OLM) studies were applied for characterization of both freely suspended and extracted carbon particles (CP) precipitated on various substrates: glass, quartz, Si and Cu.

It was shown that each precipitate is heterogeneous; it contains separated randomly padding particles, their aggregates and self-assembled ensembles of particles. We conclude that ensemble of particle consists of large particle those posses graphite structure and some quantity of graphene – type dots (flaks).

The conclusion was made that large particles reveal bulk graphite Raman spectra, while small particles show Raman properties of multilayered graphene. Synthesized carbon nanomaterials reveal interesting optical features and at the same time, we can state that luminescence study is a very useful analytic tool for investigation of the structure and physical properties of micro- and nano- sized carbon materials, e.g. of graphene like carbon dots.

Tunable frequency nanolaser

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In the field of optical spectroscopy of molecules and crystals is always urgent task of creating a source of coherent radiation with a narrow radiation line tunable over the entire visible wavelength range. Currently, this problem is successfully solved with the aid of tunable lasers.

The purpose of this paper is to discuss the possibility of frequency tuning in the optical domain using methods of nanoplasmonics. It will discuss new opportunities on the example of so-called plasmonic nanolasers. Their dimensions are, by definition, much smaller than the wavelength of the optical radiation and should not apply the frequency tuning techniques are used for lasers having macro- or microsizes. The fact that nanolaser oscillation frequency is determined by the phenomena of metallic nanoparticle plasmonic resonance. For well-conducting metals (such as gold, silver, platinum, etc.) the frequencies of oscillation of the free electron gas for such metal nanoparticles just get in the visible and near infrared range. The frequency of the radiation of a single nano-emitter can be varied depending on the size, shape and structure (e.g., nanocomposites different topology), and other factors. In currently implemented two-dimensional sets of nanolasers great influence on the radiation frequency has interaction between the individual nano-emitters.

On concrete examples we describe our new ideas to transform the eigen-frequency nanoplasmonic structures and nanocomposites: namely, the use of quantum mechanical superposition related plasmon oscillations (for example, in case of nanoring); quantum interference of continuous and discrete spectra transitions (Fano-like plasmonic resonances), in particular, quantum interference of two closely spaced plasmonic resonances, for realizing extremely narrow plasmonic line. It will be an example of effective use of nonlinear wave mixing in plasmonic nanostructures for smooth frequency tuning. New nanomaterials as nanorubber and piezo-nanoceramics will be discussed. We hope that these new ideas and materials will help to find new routes to create elements trasformation optics.

Fabrication, morphology and optical properties of some transparent oxide ceramics

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The transparent optical ceramics is very perspective objects for research. They can be used instead of classical optical materials (i. g. glasses, crystals), and as brand new materials. Simple fabrication, possibility of comprehensive composite structures creation, better optical and physical properties are their advantages. In last decade, transparent optical ceramics are finding wide application as an active media for lasers, passive Q-Switch, windows, etc.

We have investigated the yttrium-aluminium garnet doped with neodymium and ytterbium rare-earth ions. These ceramics were made with reactive sintering method and the series with different concentration of activators, different sintering temperatures and different time of sintering were got. The morphology of the samples was investigated by atomic-force and optical microscopy. The optical, photoluminescence and lasing properties were found.

The second object of our research were the glass-ceramics of the lithium germinate (Li_2O-xGeO_2, $x = 7, 11.5$). The samples were prepared with fast sintering method. The different phases: glass, glass-ceramics and poly crystals were got. Their morphologies were investigated using atomic-force microscopy.

The optical, photoluminescence and X-ray luminescence properties were measured in detail and obtained results were discussed.

New luminescent probes for ROS detection based on CeO_{2-x} nanocrystals

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Problem of the control of the concentration of reactive oxygen species (ROS) in the living cells nowadays has attracted a lot of attention in the biological and medical communities.

It is widely accepted now that cerium dioxide (CeO_2) nanoparticles due to their unique ability to spontaneous regeneration of antioxidant properties present one of the most perspective classes of redox-active materials for treatment of the negative consequences of an oxidative stress determined by action of reactive oxygen species (H_2O_2, O_2^-) in a living cell.

In our work, we have investigated at first the possible application of cerium dioxide as luminescent probe of ROS concentration. We have observed that CeO_2 possess effective luminescence properties with luminescence caused by the radiative relaxation in two different optical centers: the first one is Ce^{4+}-O^{2-} charge transfer state and the second one – Ce^{3+} ions [1]. The ratio of Ce^{4+}/Ce^{3+} centers depends on the content of oxygen vacancies; therefore, the variation of ceria stoichiometry allows changing the concentration of Ce^{4+}-O^{2-} and Ce^{3+} luminescence centers [2]. As was shown before, content of Ce^{3+} ions in CeO_2 determines also the antioxidant properties of this material, so intensity of Ce^{3+} luminescence can be used as a measure of antioxidant ability of ceria nanocrystals obtained by different routes.

This fact along with high sensitivity of Ce^{3+} intensity to interaction with oxidant also shown in our studies provides a unique possibility of the visualization and control of the dynamics of ROS neutralization by CeO_2 nanocrystals in the living cell by the methods of optical spectroscopy.

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Inorganic NPs as a platform for controlled intracellular delivering of hydrophobic cargo

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One of the most research area of nanotechnology is nanomedicine, in particular, tissue- and cell-specific drug delivery. Nanomedicine focuses on formulation of therapeutic agents in biocompatible nanocarriers (NCs), such as lipid vesicles, micellar systems, nanocapsules, dendrimers, biopolymers and inorganic nanoparticles (NPs).

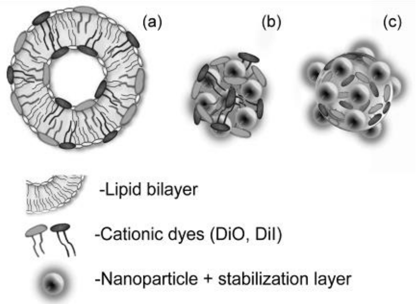

Fig. 1. Schematic representation of PC liposomes/dyes (a) NPs/dyes (b) and NPs/dyes/cholesterol complexes

Despite the rather wide applications of inorganic NPs as therapeutic, diagnostic and imaging agents, their application as a nano-scale platform for nanodrug development is still under study. In recent years some NPs, i.e. nanocrystalline ceria and rare-earth doped orthovanadate NPs have revealed high biological activity (oxidative stress prevention, anti-inflammation and neuroprotective activity, antitumor effect) that attracts a lot of interest to these objects as a platform for design of multi-functional drug with the synergetic effect.

In the present study, the efficiency and kinetics of NCs/dye molecules complexes accumulation in living cells and dye release have been studied using fluorescence microspectoscopy and FRET-labeling of various nano-scale carriers: organic liposome vesicles and inorganic nanoparticles (CeO_2 and $GdYVO_4:Eu^{3+}$). NCs/dyes complexes formed in aqueous solutions have been characterized. It has been shown that NCs based on $GdYVO_4:Eu^{3+}$ nanoparticles exhibit the most effective accumulation in cells and provide very fast release of the lipophilic cargo (dyes molecules). Lipophilic compound (cholesterol) embedded into the NCs/dyes complexes decreases noticeable the rate of lipophilic dyes release and reduces the affinity of the complex interaction with hepatocytes. $GdYVO_4:Eu^{3+}$ NPs could be used as a nano-scale platform for controlled intracellular delivering of hydrophobic agents.

Viscosity of nano-fluctuation critical fluid taking into account the spatial dispersion of the system

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Now in connection with the wide practical use of the unique properties of the substance under critical condition in the novel technologies [1] the interest in experimental and theoretical studies of the properties of the critical fluid is significantly increased. This applies particularly to the kinetic properties of substance such as diffusion coefficient and viscosity.

Three-dimensional surfaces of the critical viscosity have been constructed for isobutyric acid - water solution near the stratification critical temperature based on the dynamic theory of critical phenomena [2], as well as on the critical viscosity equation [3], which takes into account the spatial dispersion of the system near the critical point [4]. Based on these results the range of applicability of these qualitatively different equations of critical viscosity has been determined.

The results of the concentration and temperature dependences of fluctuation part of viscosity confirm the form of the viscosity equation that takes into account the spatial dispersion of the system over the range of temperature $t \approx 10^{-4} \div 10^{-2}$ and concentration $x = 0 \div 0{,}5$.

Equations of the critical viscosity based on dynamic theory of critical phenomena [3] and taking into account the spatial dispersion of the system [4] are consistent with each other and with the experimental results only in a narrow range of concentrations near the thermodynamic critical iso-contsentrate direction in the temperature range $t \approx 10^{-4} \div 10^{-3}$.

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Photoluminescence of Rhodamine 6G in plasmonic field of Au nanoparticles: temperature effects

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Influence of temperature on the photoluminescence of rhodamine 6G deposited on 2D array of the gold nanoparticles was studied in the temperature range of 78–278 K [1]. The PL from R6G on Au NPs array is enhanced by the coupling of exciting and emitted photons to the surface plasmons excited in the NPs. There is a significant difference in the temperature behavior of the PL spectra from R6G–Au and R6G samples. The ratio of PL intensity of R6G on Au to one of R6G without Au was found to be monotonically decreasing with temperature. This indicates the fact of monotonic decrease of the factor of plasmonic enhancement of PL from R6G on Au NPs with temperature. The theoretical model was proposed to explain the observed temperature dependence of plasmonic enhancement factor. Where electron-phonon scattering and thermal expansion of the gold nanoparticles were considered as two competing physical mechanisms of the temperature dependence of plasmonic enhancement factor. The calculations of the influence of temperature on the PL spectrum of R6G in plasmonic field of Au NPs were performed. The results of calculations agree with the results of the experimental observations. The calculations showed that the electron-phonon scattering is prevailing mechanism in the temperature dependence of the factor of plasmonic enhancement of PL from R6G on Au NPs as compared to effects related to the thermal expansion of Au NPs.

The temperature induced increase of the scattering rate leads to higher plasmon damping that causes the decrease of plasmonic enhancement of rhodamine 6G luminescence.

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Transmission and inelastic scattering in synthetic opals filled with KH_2PO_4 nanocrystals

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The obtaining and investigation of nano-sized nonlinear optical crystals attracts a great attention in solving applied problems of nolinear optics. In case of periodical arrangement of nanocrystals, new effects should be expected due to the additional interference of nonlinear waves. This work is devoted to working out the KH_2PO_4 (KDP) embedding procedure in pores of synthetic opals and to characterizing the samples by optical spectroscopy methods.

An embedding procedure was a soaking of initial opal into a water- KDP solution at about 50 ^{0}C with the following crystallization by evaporating the solvent. Optical spectra were measured by using laser spectrometer on the base of double monochromator DFS-12. Inelastic scattering spectra excited by a 532 nm DPSS laser were recorded in different scattering geometries.

The opal-KDP transmission spectra demonstrated the broadening of the ‘non-transmission’ band caused by the Bragg diffraction on the (111) planes of initial opal. The diminishing of its depth by increasing KDP concentration in opal was due to the decrease of optical contrast. The additional prove of the KDP embedding was a more broadened band at 916 cm^{-1} in KDP-opal Raman spectrum that is typical for the KDP single crystal spectrum. Besides, a wide intensive band was observed within a 0 – 1200 cm^{-1} range. The tail of this band in the anti-Stokes region is not satisfactory described in terms of Raman scattering processes. Such inelastic scattering may be connected with the parametric processes.

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The study of effective excitation conditions of rhodamine 6G molecules in synthetic opal

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This work is devoted to searching for the optimal conditions of the rhodamine 6G (R6G) excitation with the aim of the further application of “opal - laser dyes” systems in random lasing.

Synthetic opals with a different grade of structure disordering are soaked in a R6G – ethanol solution (10^{-4} and 10^{-5} M). A 532 nm DPSS laser and a 517 nm LED radiation are used for the excitation. The spatial distribution of the R6G emission spectrum is obtained by scanning the excitation radiation through the sample. A stability of dye molecules under the long-time (50 min) laser excitation is studied. The effect of internal and external metallic (copper and silver) resonators on the R6G emission efficiency is also investigated.

Emission spectrum of laser dye in synthetic opal pores is defined by spectral position of photonic stop-band, by spatial distribution of dye molecules, and by spatial distribution of structure defects. The defects may cause an additional scattering of the exciting and/or emitting photons and result in photon localization. Excitation geometry should be also chosen in a proper way to diminish the re-absorption. The most preferable excitation conditions are found to be the right angle geometry by focusing the exciting radiation into the 0.7 mm thickness layer near by the (111) surface. The existence of internal silver resonators together with the structure disordering may raise the R6G emission efficiency in several times.

This work was supported by the project “Capture of electromagnetic emission in resonance structures and in resonance photonic crystals with luminescent centres”.

Spectroscopic studies of Ar clusters generated in a supersonic jet

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VUV luminescence spectroscopy is a powerful tool for investigating the final step of the relaxation of electronic excitations in rare gas clusters [1].

In the present work, we study the VUV cathodoluminescence spectra of Ar clusters produced in supersonic jets expanding into a vacuum. The measurements were performed at a stagnation pressure P_0 = 0.1 MPa and stagnation temperatures T_0 varying from 150 to 500 K. An electron beam with an energy of 1 keV and current of 20 mA excited the supersonic jets. The resulting emission was spectrally dispersed by a monochromator and registered by a channel multiplier VEU-6. In the 50-110 nm wavelength range of the spectra measured in the atomic and cluster regimes of jet flow, we observed lines of singly ionized argon and resonance lines emitted by the excited atoms. For a number of the identified ion lines λ=637Å, λ=919Å, λ=932Å, we obtained dependencies of their intensity on the amount of matter condensed in the jet.

The analysis of the dependencies confirms the assumption that the curve peculiarities reflect the changes in the jet composition during the gas condensation. A high-temperature plateau in the dependency of the line λ=637Å suggests that the jet consists of atoms. The decrease in the line intensities with lowering stagnation temperature is indicative of cluster formation and can thus be used to estimate the amount of the condensed matter and the number of clusters in the jet.

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Metamorphic InAs/InGaAs quantum dot structure: photoelectric study

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The photoluminescent and photoelectric properties of InAs quantum dots grown on an $In_{0.15}Ga_{0.85}As$ metamorphic buffer are studied.

The structure shows an efficient photoluminescence signal at 0.93 eV and a weak band by the InAs wetting layer near 1.2 eV at room temperature, the bands shift to 1.02 and 1.26 eV respectively being cooled to 10 K. Spectral position of the quantum dot emission corresponds to the telecom window at 1.3 µm (0.95 eV).

The structure with vertical contacts is found to be photosensitive in the spectral range above 0.9 eV at room temperature. All the components of the structure from quantum dots at 0.9 eV to the metamorphic buffer above 1.22 eV are observed in the photovoltage and photoconductivity spectra. The indirect effect of GaAs manifests itself as only with the drop of the signal at 1.36 eV. No effect of defect centers on the photoluminescence and photoelectrical properties is found, although they are observed in the absorption spectrum. The band structure provides a good collection of charge carriers to the InAs quantum dots which leads to high photoluminescence signal.

These results confirm that the proposed metamorphic quantum dot structure is a viable option for the development of optoelectronic devices, as the presence of defects due to strain relaxation of the metamorphic buffer does not forbid an efficient collection of carriers into quantum dots.

Dynamics of Frenkel excitons in molecular J-aggregates formed in nanostructured anodic aluminum oxide

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Development tendencies of new optical materials for photonics and optoelectronics show that the investigation of organic luminophores properties is very actual nowadays [1]. Very perspective objects in this direction are well-ordered molecular nanoclusters called J-aggregates. Formation of J-aggregates in pores of anodic aluminum oxide (AAO) which demonstrates strict ordering of pores at large surface areas, narrow dispersion of pore diameters and the intervals between them, perfect cylindrical shape and the strictly parallel channels seems to be the most attractable. Mathematical treatment of the AAO samples has shown that the average pore diameter is 42 ± 4 nm and the distance between their centers is 83 ± 2 nm [2].

The goal of this work is to determine the exciton transport parameters for J-aggregates formed in AAO samples. In addition, we used J-aggregates with different structures: spherical BIC J-aggregates with an average diameter about 20 nm and thread-like PIC J-aggregates with a length up to 10 microns and a diameter of 2.3 nm. To investigate the exciton migration efficiency in J-aggregates we used cyanine dye DiD as an exciton trap.

As a result, the excitons in spherical J-aggregates are revealed to migrate over 120 BIC molecules and in the case of thread-like J-aggregates – over 150 PIC molecules. Such exciton transport efficiency is much higher in AAO samples as compared to that for the J-aggregates formed in solutions.

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Thermoluminescense study of poly (di-n-hexylsilane) film and nanocomposites

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The study of low temperature thermostimulated luminescence (TSL) provides important information about the presence of traps and defects for charge carriers in silicon organic polymers that are promising materials for transport and luminescent layers in electro-optical devices.

We carried out comparative TSL study of the PDHS film and nanocomposites in the temperature range of 5–120 K. The PDHS/MCM-41 and PDHS/SBA-15 nanocomposites were prepared by introducing polymer into nanoporous silica with different pore diameters (2.8 and 9 nm) respectively. It was shown, that changing the pore size we can vary the number of traps and investigate the charge localization depending on confinement effect.

It was found that TSL curve of the PDHS/MCM-41 composite shifts to lower temperature by 33 K comparing to that of the polymer film. It shows the structure consisting of two bands: narrow band with maximum at 17 K and weaker broader band at 28 K. TSL curve shows distribution of traps in the polymer. There is only single polymer chain inside the pore diameter of 2.8 nm. In this case, TSL curve must be significantly shifted to lower temperature comparing to TSL curve of polymer film, and it is observed experimentally. We assume that the band at 17 K is associated with the charge release from traps (oriented segments), and the band at 28 K corresponds to defect states.

TSL curve of the PDHS/SBA-15 composite shifts to higher temperature comparing to TSL curve of the PDHS/MCM-41 composite. It has maximum at 25 K and shoulder at 35 K. Its intensity and half-width increase significantly comparing to TSL curve of the PDHS/MCM-41 composite.

Dependence of optical absorption spectra from the thickness, concentration, and temperature of $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ nanofilms

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The swift development of technologies for studying and obtaining the desired physical properties of low-dimensional heterostructures, which is observed for recent decades, is related with unique features of these systems that are the base for creation of up-to-date facilities in opto- and nanoelectronics. The most known structures used with this purpose are those based on the $GaAs/Al_xGa_{1-x}As$ heterostructures. They serve for creation of low-threshold lasers capable to operate at room temperature, highly-efficient photodetectors, light emitting diodes, re-switchers, quantum cascade lasers and detectors [1]. Despite the fact, that optical properties of such structures have been studied rather well, respective investigations are continued till now (see, for instance, [2]).

This report represents the results of theoretical investigation of the optical absorption spectra transformations by changing the thickness, concentration, and temperature of flat nanofilms $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$. Spectral dependence of absorption coefficient of the interband transitions and exciton excitation for various directions of light propagation and polarizations has been calculated. Computations was carried out by using the model of single rectangular quantum well of finite depth, the dielectric continuum approximation, and the Green's function method. It is shown that the temperature-induced variations of absorption band are invoked by the electron-phonon interaction with confined modes of phonons in nanofilms thicker than 30–40 nm, or interface ones, if they are thinner. Calculations of this type are made the first time.

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The vibrational-electronic relationship in the IR spectra of nanodiamond and bentonit

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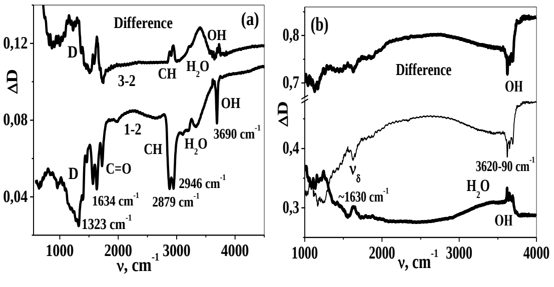
The attenuated total refraction (ATR) and diffuse reflectance (DR) FTIR spectra of the detonation nanodiamond (ND) (ALIT, s. Biysk and other) and bentonite $Al_2[Si_4O_{10}](OH)_2 \cdot nH_2O$ have been studied. The anomalously strong change of the background intensity in the broadband DR spectra was found. It is well manifested in the difference spectra shown in Fig. (a), (b). Also it is significant that with the strengthening of the background of the ND vibrational bands D~1330 cm^{-1} and functional groups CH, OH, C=O and water its shell in most cases attenuated (fig.(a),(b)). The observed radical change of the spectra can not be attributed only to the influence of the multiple scattering of the light (MSL). It was associated with the emergence of new electronic states (NES) and observed new bands with half-width δν from 50 to 1000-th cm^{-1}. The existence NES confirmed by the observation of their ATR spectra where no influence of the MSL.

The NES is observed at infrared active vibrations. This is indicates a vibration-electronic relationship (VER). The comparison of the ATR and DR spectra has revealed differences of functional groups on the surface and inside the ND agglomerates. For example, in the ATR FTIR spectrum have been observed ~ 30 different OH groups, but in DR spectra only two lines 3670 and 3692 cm^{-1} are amplified about 60 times. It found a difference of the molecular states of the water inside and on the surface of the ND agglomerates. For the first time, it was observed vibration bands of negative polarity, for example, CH_2 and CH_3 groups in ND absorption spectra (glow) on the background of the NES positive bands. The abnormally strong VER in the nanostructures has allowed clearly observe the complex overtone band ND 4D with a sharp peak around 5311 cm^{-1} and different bands 2D and 4D for the various type of the ND.



Aging effect of gold sols synthesized in aqueous solution of branched Polyacrylamide

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Last time gold nanoparticles (AuNPs) are of great interest for research in the field of targeted drug delivery. Nanosystems with high content of AuNPs may increase efficiency of drug as well as reduce side effect of toxic anticancer agents. On the other hand, aqueous AuNPs have to be stabilized because of disposition towards aggregation. Polymers of different macromolecular structure are extensively used to stabilize such nanosystems as well as to increase drug capacity.

Current work is dedicated to the study of aqueous AuNPs, synthesized by in situ reduction in the presents of branched copolymers Dextran-graft-Polyacrylamide (D-g-PAA) of different macromolecular architecture (variable number of PAA arms), linear Polyacrilamide and its anionic derivatives. Facile chemical approach has been chosen to reduce metal ions from their salts, widely studied reducing agent Sodium Borohydride ($NaBH_4$) were used to fabricate AuNPs. Special emphasis was placed on the aging effect in these systems, namely, size changes of AuNPs during 3 months. The storage stability of Au sols was studied by transmission electron microscopy (TEM), dynamic light scattering (DLS) and UV-vis spectroscopy. It was observed that the most significant changes of AuNPs size distribution take a place during the first month of observation. Average nanoparticles size changes from 4-8 to 10-12 nm and the aging process depends on polymer matrix type according. Moreover, it was proved that size distribution and the aging process is strongly depending on the nature of polymeric stabilizer. Branched polyelectrolyte matrices allow to synthesize AuNPs with higher content of small particles (4-5 nm) while it was impossible to synthesize stable sol in the case of linear anionic PAA. It should be noted that the size data received by DLS and UV-vis spectroscopy are in compliance with TEM image statistical analysis.

The energy spectrum of the phonon and electron states in bilayer graphene

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There were built dispersion curves of electron and phonon excitations in the high-symmetry directions of the Brillouin zone of bilayer graphene. Phonon energies were experimentally determined from the Raman spectra. Computer calculations of the structure of the electronic bands and analysis of symmetry for states with excitation wave vector $\mathbf{k} \neq 0$ were performed.

Compatibility relations for projective representations for all directions in Brillouin zone have been defined. It was shown that the spin-orbital interaction leads to a splitting of the doubly degenerated electronic states in K-points.

Optical Properties of CdS Nanoparticles Synthesized in Star-Like Dextran-Graft-Polyacrylamide Matrices

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Nanoparticles have attracted great interest in recent years because of their unique chemical, physical, optical, electrical and transport properties which are different from those of either the bulk materials.

In this paper we report a simple chemical precipitation synthesis route at room temperature using star-like dextran-graft-polyacrylamide matrices.

CdS nanoparticles have been prepared by coprecepitation method in aqueous solution of graft copolymers Dextran-Polyacrylamide (D-g-PAA). Dynamic light scattering evaluated to this nanosystems shows the existence of both CdS nanoparticles (15 nm) and macromolecules of D-g-PAA (70 nm).

The photoluminescence emission spectra of the synthesized CdS nanoparticles at excitation wavelength 400 nm exhibits two broad bands centered at 536 nm and 567 nm. The band corresponding to 536 nm provides Green emission while band at 567 nm gives Yellow emission. The Green emission band was associated with the emission due to electronic transition from the conduction band to an acceptor level due to interstitial sulfur(IS). The Yellow emission was attributed to recombination via surface localized states, a transition from interstitial cadmium (ICd) to valence band.

UV-Vis absorption spectrum of the CdS nanoparticles shows the blue shift in absorption edge compared with bulk CdS.

Optical properties of $(Ag_3AsS_3)_{0.6}(As_2S_3)_{0.4}$ thin films prepared by PLD technique

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The present investigation is aimed at the spectroscopic studies of optical transmission and absorption spectra as well as the refractive index dispersion of $(Ag_3AsS_3)_{0.6}(As_2S_3)_{0.4}$ thin films at different temperatures.

Synthesis of $(Ag_3AsS_3)_{0.6}(As_2S_3)_{0.4}$ composite material was carried out at a temperature of 700°C for 24 h with subsequent melt homogenization for 72 h. $(Ag_3AsS_3)_{0.6}(As_2S_3)_{0.4}$ thin films were prepared by pulse laser deposition (PLD) technique. The film thickness was measured using an Ambios XP-1 profile meter.

The optical transmission spectra were studied in the interval of temperatures 77–300 K. With temperature increase the longwave shift of high-energy parts of transmission spectra and transmittance decrease at interference maxima are observed. Based on the interferential transmission spectra, the spectral dependences of absorption coefficient were obtained. It is shown that the optical absorption edge in the region of its exponential behaviour are described by Urbach rule. Temperature dependences of optical pseudogap and Urbach energy for $(Ag_3AsS_3)_{0.6}(As_2S_3)_{0.4}$ thin film are well described within the framework of Einstein model. Urbach absorption edge parameters as well as the temperature dependences of optical pseudogap and Urbach energy are determined.

The dispersion dependences of the refractive index for the thin films were obtained from the interference transmission spectra. The slight dispersion of the refractive index is observed in the transparency region while it increases when approaching to the absorption edge region. It is shown that at temperature increase the refractive index increase.

Phosphine Derivatives Stabilize CdSe Nanoclusters

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Ultra-small clusters of III-V semiconductors are usually used for a communication, information technology, medical devices and biological studies. The small size which numbered tens of atoms provide high sensitivity to the pH values and dielectric permittivity [1,2]. On the other hand, nanoclusters (NCs) exhibit low quantum yield. In order to improve stability and brightness we have used the derivatives of phosphine as additional surfactant. Absorption (Abs) and Photoluminescence (PLs) spectra of the $CdSe_{33,34}$ NCs in the toluene by itself and in the presence of phosphine's have been studied. Freshly prepared NCs have been mixed with triphenylphosphine (TPP), trioctylphosphine (TOP) and tris (pentafluorophenyl) phosphine (TPFP). Concentration of the additional surfactant in the range of 50-200 mM have been chosen according to the 300 mM concentration of main surfactant octylamine. It has been observed that TPP and TOP at 100 mM concentration can stabilize NCs and increase the brightness of NCs up to 90% compare to the control sample without phosphine. They can bind to the surface of NCs and help to stabilize NCs in the dilution. Mixture of the NCs with TPP and TOP have been kept for a few hours in diluted and non-diluted probes and measured after each two hours. TOP and TPP revealed stabilization effect both for diluted and non-diluted samples even after 24 hours. TPFP have exhibited strong destabilization effect and almost no gain in the brightness.

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Classic and modulation spectroscopy of C_{60} fullerene heterostructures

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The discovery of new carbon cage molecules C_n called fullerenes led to a new class of carbon-based solids and heterostructures. At the moment, in accordance with literary data, C_{60} solid energy gap value dispersion is of 1.43 eV to 2.35 eV, and the type of lower electron junction (direct or indirect) was not determined yet. Heterostructures were produced from C_{60} fullerene beam by thermal vacuum sublimation onto non-heated silicon, quartz, mica and glass substrates. The effects of the film deposition conditions and type of substrate on the heterosystructures properties were established. If the films deposition velocity increased, the new carbon phases (graphite- or diamond-like) formed in the films. Crystalline structure, composition, optical and electron properties, internal mechanical stresses in the heterostructures were studied by classic optical methods and modulation spectroscopy.

We have measured light absorption and reflectance, Raman, Fourier, photoluminescence, modulation electroreflectance spectra, and too the heterostructures bending. The electroreflectance spectra were measured by an electrolytic method in the spectral range 1.5… 3.6 eV. Important experimental data were obtained about the film and interface, their structure perfection, optical and electron properties: band gap, electron junction and conductivity type, the charge carries scattering, the mobility and the time of the energy relaxation of light exciting charge carries, Franz-Keldysh effect in a built-in electric field and surface size quantization of the electron energy in the electron enriched fullerene surface in interface.

It was established that C_{60} solid is direct-gap semiconductor with about 1.6 eV band gap (E_0) in the singular X point of the Brillouin zone. The next direct transitions in this point were observed in spectral range about 2.2 eV and 3.5 eV. The films band gap depended on inner mechanical stresses. We calculated the value of this dependence on the basis of the data on electrorefletance spectra and the heterosystem bending.

The value - $2.8 \cdot 10^{-10}$ eV/Pa was obtained for E_0 transition in solid C_{60}.

Effect of acid treatment on the microstructure and physical properties of multiwalled carbon nanotubes suspension in glycerol

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The effect of acid treatment on the structure and properties of suspensions of multiwalled carbon nanotubes (MWCNTs) in glycerol has been investigated. The concentrations of MWCNTs were within 0-2% by weight. Suspensions were treated during 5-60 min at T = 343 K by a mixture of concentrated nitric and sulphuric acids with the volume ratio of 1:3. The degree of acid treatment influence on the structure of suspension was analysed using methods of thermal analysis and infrared spectroscopy. For oxidized samples beginning of thermal degradation is observed at significantly lower temperatures than for the original sample. This is reflecting the presence of disordered or amorphous carbon at acid destruction NT. Thermogravimetric data indicate an increase in the degree of destruction of NT with increasing treatment time from 5 to 60 min. IR spectroscopy data indicate a significant increase in the concentration of COOH and OH groups on the surface of NT due to acid treatment. By increasing the degree of acid treatment also observed significant visual change in the structure and size of clusters NT in suspension of glycerol. In all cases, both the untreated and acid -treated NT, there was a pronounced electrical percolation behavior. However, acid treatment resulted in a significant decrease in conductivity, σ, suspensions and significant enhancement of the temperature dependence of σ. Oxidation of MWCNTs could affect significantly their thermal stability and degree of destruction.

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Raman spectrum of bismuth tellurite nanocrystals grown in synthetic opal pores

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The present work is devoted to a growth of bismuth tellurite (Bi_2TeO_5) nanocrystals in pores of synthetic opal and to study manifestation of the structural changes and the size effects in Raman spectrum. The Bi_2TeO_5 crystals are a photorefractive material with high photorefractive sensitivity and a long living photorefractive signal [1].

Filling of the synthetic opal pores with the average linear size of 70 nm was carried out by melting of Bi_2TeO_5 thin crystal plate ($T_m = 900^0C$) which was placed on a surface (111) of the synthetic opal sample. The furnace temperature was about 1030°C.

The Raman spectra of the Bi_2TeO_5 crystal and the nanocomposite opal-Bi_2TeO_5 were measured in the back-scattering geometry. The Raman spectrum of the Bi_2TeO_5 nanocrystals in the opal pores has a number of significant variations from the spectrum of initial crystal. In order to understand the nature of the change in Raman spectra of the nanocomposite opal-Bi_2TeO_5 and check value of evaporation of TeO_2 during the crystal growth process the comparison with Raman spectra of the nanocomposites opal-$Bi_{12}SiO_{20}$ [2], and opal-TeO_2 [3], nanowires α-Bi_2O_3 [4] was made.

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Photogeneration and recombination processes in Ge-Si heterostructures with Ge nanoclusters grown on Si(001)

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In nanosize semiconductor heterostructures quantum size effects can result in changes of the electron spectrum [1,2]. The investigation of SiGe/Si nanostructures bears good prospects for the development of novel nanoelectronic devices [3].

We investigate the processes of generation and recombination of charge carriers in heterostructures with Ge nanoclusters by studying the photoconductivity spectra and by using the Kelvin probe force microscopy (KPFM).

In the photoconductivity spectra it is possible to distinguish two components. At energies greater than the band gap width for silicon, at the appropriate temperature, the main contribution to the photoconductivity is due to interband transitions in the p-Si substrate. In the spectral region, where c-Si is transparent, the photoconductivity is attributed to interband optical transitions involving the quantum confined states of the nanoislands.

The recombination efficiency of the electron-hole pairs involving quantum confinement states in nanoislands is higher in comparison with the rate of recombination of the carriers photogenerated in Si substrate. It was found that when we have selective photoexcitation, recombination of electron-hole pairs in SiGe nanoislands is defined by spatial separation of nonequilibrium charge carriers, when the holes are captured in the valence band states of SiGe nanoislands and electrons are in silicon environment.

KPFM was used for the detection of charge trapping and recombination in Ge NCs. The observation of a surface potential distribution with maxima at the Ge NC location and lowest values at the NC's surrounding is indicative for trapping of positive charges within the NCs. A clear linear decrease of the potential from the top of the Ge NCs to their bases is observed. This manifests that the number of holes stored in the individual Ge NCs is higher as compared to holes captured by other traps of the substrate surface.

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Peculiarities of Interaction of Polymethine Dyes with CdSe Nanoparticles at Low Temperatures

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Such objects of investigation, as complexes formed from polymethine dyes (PMD) and nanoparticles (NP) attracts more and more attention of researchers. The ability of many species of PMD to the aggregates formation is an important property in terms of the applied use of them. In this paper we present the experimental results of studying of CdSe nanoparticles influence on polymethine dyes (forming and no forming of aggregates Fig.1 left and right respectively) at low temperature (4K).

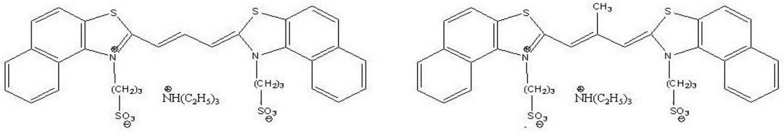

Fig. 1. Chemical formula of studied dyes.

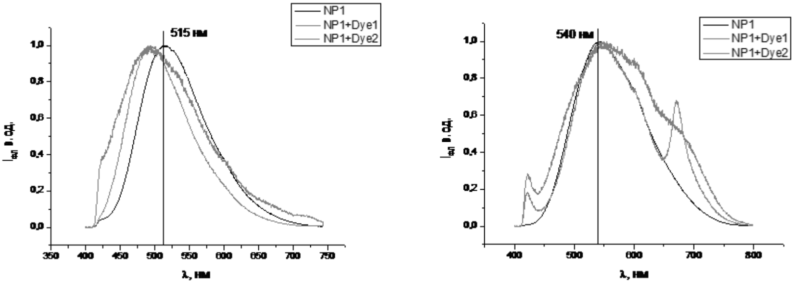

Fig. 2. Normalised fluorescence spectra of CdSe nanoparticlrs with dyes **1** (a) and **2** (b) at 4K(a) and 300K (b)

Peculiarities of Raman Spectra of Graphene-like MoS_2/C Nanocomposites

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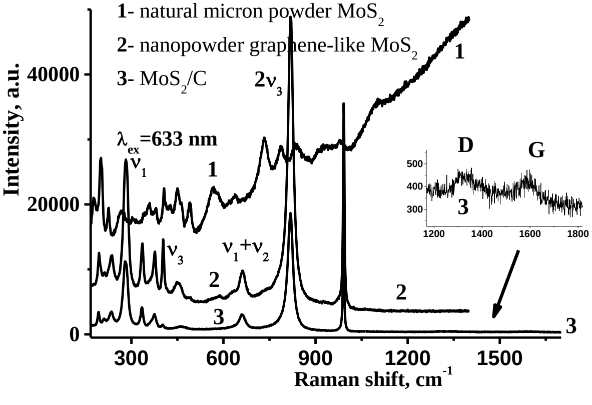
Molybdenum disulfide (MoS_2), a typical layered transition metal sulfide has an analogous structure to graphite, but due to the presence of different atoms in elementary unit cell and dipole character of vibrations manifests significantly richer Raman and IR spectra. We have studied Raman spectra (λ_{ex}= 488 and 633 nm) of MoS_2 nanocrystallites (NCs) with sizes (4-5) x20 (40-50) nm and a thickness of 6-8 layers. The effect of the addition of carbon (0.5–1%), which can intercalate MoS_2 or form monolayers of graphene on the surface of MoS_2 NCs has been investigated. Changes in the Raman spectra at the transition from micro- to nano-samples MoS_2, and an enlarged image of spectral region of D and G bands for nanocomposite MoS_2/C are shown in Figure below.



The presence of C-atoms in NCs results a change of the frequencies $\nu_{1,2,3}$ at 15÷25 cm^{-1} and a significant weakening of the overtone $2\nu_3$, as well as appearance of the electronic bands due to vibrational-electronic interaction in the field of TA-LA and $\nu_{1,2,3}$ modes. Two other Raman peaks at 1350 and 1590 cm^{-1} can be seen in the spectrum of MoS_2/C, which are related very well to the D and G bands of graphene.

“Green” Synthesis and Spectroscopic Characterization of CdS Nanoparticles

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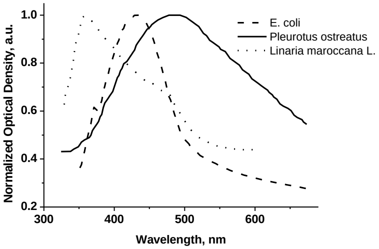
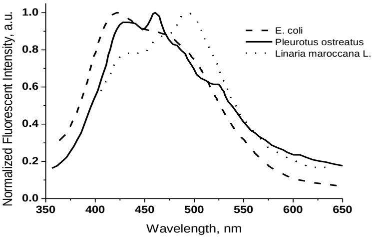
The biosynthesis of semiconductor nanoparticles (quantum dots) nowadays is a new promising field of research. These nanoparticles have a diverse range of applications, namely they can be used in biological studies as visualization probes in living cells, for pathogen and toxin detection and immunofluorescent labeling of proteins, in cancer therapy, as well as solar cells components, light emitting diodes and infrared photodetectors in optoelectronics.

The present study is the report devoted to obtaining cadmium sulfide quantum dots using the fungus *Pleurotus ostreatus, roots Linaria maroccana* and *E-Coli.*

CdS nanoparticles synthesized by us using plant extract or bacteria have typical for quantum dots optical properties such as specific absorption (left) and luminescent (right) spectra.





Optical and ultrasound spectroscopy of micro/nano cellulose incorporated with complex oxides

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Now, various cellulose derivatives are widely used in many fields of people's activity and beside they under intensive studies. So, the perspectives of the cellulose usage spread from "paper electronics" to forensic examination and eco-friendly sorbents. Optical and luminescent properties of the cellulose have been known for many years, but in spite of the fact that cellulose demonstrates intensive own luminescence, cellulose was not used anywhere as optical material, particularly for detecting of ionizing radiation: UV, VUV, X-ray, etc. material. That situation is mainly related with destruction of cellulose body under ionizing or UV irradiation. The destruction factor is not so important for micro/nanosized cellulose (MNC) as its body cellulose is constructed from macro-chains.

This work presents the results of morphology and physical (especially luminescent) properties study of the body and surface of the MNC samples made by us. Several types of the "pure" and embedded with luminescent inorganic oxide dielectric micro- and nanoparticles cellulose composites were prepared and studied. There were thin disks pressed from: a) initial micro/nano cellulose (MNC) powder; b) mixture of MNC and luminescent inorganic oxide dielectric powders like to La/Bi phosphates/vanadates doped with some luminescent RE ions (Eu^{3+}, Sm^{3+}, e.g.) Some of the samples were undergone to carbonization via temperature treatment in the range 50 – 230^0 C.

Morphology of the samples surfaces was monitored using optical and electronic microscopy. Photoluminescence characteristics were also measured. Some related characteristics were measured too. There were dielectric permittivity and specific heat capacity those were measured in the wide region of fixed frequencies of ultrasound waves and various temperatures of the samples.

The relations between content and structural, electric, thermo and luminescent characteristics of the cellulose composites are discussed.

Interface interaction effects on the electro-optical properties of nanocomposites: LC 5CB –montmorillonite (MMT) natural aluminosilicate particles

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Physical properties of the heterosystems “nematic liquid crystals - anisometric nanoparticles” are of great interest, because these materials can be used in the development of modern optical devices. The type and strength of interphase interactions between the components affect electro-optical (EO) properties of the samples. Our EO studies of the composites: 5CB – montmorillonite (MMT), modified by different surface-active substances (SAS), show that EO “memory” and contrast are dependent on an affinity degree of the nanoparticle surface to the molecules of the organic medium.

In this work we investigated LC 5CB, filled with MMT from three deposits (Askan, Pyzhevsk, Cherkassy). According to IR-spectroscopy data, narrowing of bands assigned to the vibrations of bonds in a crystal lattice of MMT and in 5CB dimers indicates Van-der-Waals interactions between the components, resulting in the alignments of molecules on a phase separation boundary. Interaction strength was found out to depend on the MMT type.

The largest EO “memory”, M, is observed in the system with the strongest affinity: Askan MMT possesses M=69%, and Cherkassy one has M=29%. The affinity degree between the components determines the composite structure, which is the most homogeneous in the heterosystem with the strongest interphase interactions. The strength of these interactions can be controlled by changing not only the chemical content of SAS, but also physico-chemical properties of MMT, and the composites with a wide range of EO parameters can be obtained.

The work was fulfilled under the financial support by NASU, the Project V153.

Surface-enhanced Raman spectroscopy for Ag nanoparticles/indocyanine dye composites

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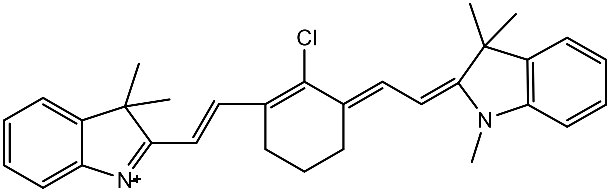
Relevant work is dedicated to the use of nanostructures based on Ag nanoparticles and indocyanine dye in photodynamic therapy of cancer. The creation of such nanostructures requires implementation of complex fundamental and applied physics investigations, aimed to study the principles and practices that ensure, in particular, the possibility of efficient energy use of in terms of the biological environment.

Ag nanoparticles are widely used in a spectrally selective coating for absorbing solar energy, as catalysts of chemical reactions to antimicrobial sterilization, photodynamic therapy of cancer etc.

Indocyanine dyes are widely used in medical diagnostics. They are used for determining cardiac output, hepatic function, and liver blood flow, and for ophthalmic angiography.

In our work we used indocyanine dye showed at fig.1. It has a peak spectral absorption at about 770 nm. These infrared frequencies penetrate retinal layers, allowing angiography to image deeper patterns of circulation.



2-((*E*)-2-((*E*)-2-chloro-3-(2-((*E*)-1,3,3-trimethylindolin-2-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-3,3-dimethyl-3 *H*-indole

Fig. 1. Chemical structure of used in our work indocyanine dye.

Colloidal suspensions of Ag nanoparticles/indocyanine dye composites where characterized by absorption spectroscopy in the visible and ultraviolet regions, transmission electron microscopy (TEM) and surface-enhanced Raman spectroscopy.

Microstructure peculiarities of nanographite

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As is known one of the graphenelike structure obtaining methods is chemical treatment of layer carbon materials, for example nanographite or thermoexfoliated graphite, 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. 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 50nm with small number (less than 10) of flawless layers. The treatment of initial nanographite with less strong oxidizers leds to the formation of ribbonlike highly defective nanocarbon structure.

The effect of oxygen stoichiometry and nanocrystal size on the luminescence properties of CeO_{2-x} nanocrystals

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For a long time, cerium dioxide (CeO_2) has been widely used in high-tech industries, e.g., gas sensors, catalysis, UV, and electrochromic coatings, etc. However, recently many researches were focused on nanocrystalline CeO_2 due to possible applications in the field of electroluminescent devices, integrated optics and in biomedicine [1] Antioxidative properties of CeO_2 nanocrystals allow to use this material in the wide range of biomedical applications [2, 3].

CeO_2 has fluorite-type structure with face-centered cubic lattice. Nonstoichiometric oxides (CeO_{2-x}) are characterized by disordered arrangement of oxygen vacancies. Oxygen nonstoichiometry defines basic biomedical properties of cerium oxide - the ability to participate in redox processes taking place in the organism [4]. Literature data on the structure and properties of nanosized CeO_{2-x} often contradict each other. Moreover, most of the properties of nanocrystalline CeO_{2-x}, remain almost unexplored.

CeO_2 nanocrystals with various degrees of oxygen stoichiometry have been investigated by means of luminescence spectroscopy techniques. It was shown that luminescence of CeO_2 is determined by two optical centres of different nature: The first one is Ce^{4+}-O^{2-} complex and the second one is Ce^{3+} ion. The ratio of Ce^{4+}/Ce^{3+} centres depends on the amount of oxygen vacancies; therefore, the variation of ceria stoichiometry allows changing the concentration of Ce^{4+}-O^{2-} and Ce^{3+} luminescence centres. Luminescent characteristics of optical centres in nonstoichiometric CeO_{2-x} nanocrystals have been investigated. Investigation of splitting of Ce^{3+} 4f-5d luminescence excitation band has shown that reduction of Ce^{4+} occurred mainly by the mechanism of oxygen vacancy formation on the nearest-neighbour position to the cerium ion. Thermo luminescent analysis showed the presence of shallow electron traps associated with oxygen vacancies.

Variation of the Ce^{3+}/Ce^{4+} ratio in CeO_2 allows control of the oxygen nonstoichiometry by luminescence properties of this material. Size dependence of oxygen nonstoichiometry for CeO_2 nanocrystalls was shown.

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Ellipsometry of etched crystal Silicon surface

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Surface of a silica crystal after chemical etching was studied by ellipsometry, atomic force microscopy and scanning tunneling microscopy.The ellipsometric parameters were measured as functions of light incidence angles at two light wavelengths 546.1 nm and 296.7 nm .The calculations based on equations for the perfect plane nonoxidated surface of refractive index and absorption coefficient numbers produces different from determined earlier values.Two surface layers models were developed for both upper layer contained chemical compounds after etching and lower layer which was responsible for the sample surface roughness.By applying Airy's formula to ellipsometric data the layers optical constants and thicknesses were obtained.The calculated silica optical constants wholly correspond with the data from literature.The lower layer thickness is similar with that obtained through scanning tunneling microscopy measurements and was equal 4.5 nm with upper layer thickness 50nm.The both layers thicknesses wholly corresponded for two wavelength used in the measurements.The obtained crystal silica optical constants as well as two surface layers constants were used to calculate silicon particles content in lower rough layer applying Maxwell- Garnett and Bruggeman equations. The obtained numbers were a little bit lower than 50%.

Nanoclusters of copper oxides

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Copper oxidation processes were studied by scanning tunneling microscopy technique. Ordered nanoscale clusters on the polished copper surface were found to be a result of thermal sample treatment. Structure of the clusters was registered with spatial resolution 0.11 nm and contained two distinct phases which were distinctly different by electrical conductivity and morphology. The clusters contain mixture of CuO, Cu_2O and copper atoms. Spatial wave functions distributions as well as spreading of bandgap edges in the nanooxidates spots were found by numerical calculations applying quantum functional density theory. Oxygen atoms embedded into copper crystal lattice resulted in distinct gaps in spatial distribution of electron density. Semiconductor electrical conductivity of the nanoclusters were analyzed from the point of view of condensed matter physics of amorphous systems. Optical properties of the different type of the clusters were evaluated taking into account Spicer theorem for density of electronic states. Dispersion curves for optical conductivity of a copper surface with oxides spots were directly calculated and compared with known spectral ellipsometric data for oxidated copper surface. The obtained results have to be taken into account for electrical contacts construction in carbon based nanodevices because the clusters dimensions are comparable with typical carbon allotropes (fullerenes, nanotubes, vertical graphene clusters).

The formation of diamond-like structure at ball-milling of graphite

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Using XRD-analysis, Raman spectroscopy (RS) and TEM, various stages of mechanical activation (MA) of graphite in an argon atmosphere are studied. A formation of intermediate onion- and diamond-like structures (DLS) in the ball-milled amorphous carbon depending on the treatment time is found. As opposed to an impact of high-energy electrons, neutrons and ions with energies of ~ 10^3-10^6 eV, the energy at MA processing is injected into material through strong elastic-plastic deformations, what is mainly connected with collective excitations rather than with the appearance of local defects. It is nearer to the strong thermal excitation, which together with the nonlinear self-compression creates the conditions for graphite → diamond transformation. Using the mill specific energy input of 2.42 J/g/s allowed to reduce essentially the time of MA.

The particular sensitivity of nanodiamond structure to laser radiation was established. So, the utilization of laser excitation power of 0.1-1 mW allowed to detect the formation of DLS in the ball-milled graphite [1] as opposed to [2]. This is confirmed by the narrowing of D- and G-bands in RS after 3.5 hours grinding, decreasing of the maxima frequencies and increasing their intensities. Reliability of DLS occurrence is also confirmed by the observation of additional bands D_k at 1120 ÷ 1240 cm^{-1} and overtone $2D_k$ corresponding to the sp^3-hybridization.

It is found for the first time the appearance of new broad electronic bands in a field of vibrational states, connected with the spatial inhomogeneity of the electron density with a period of 1-15 nm (the XRD data in the angles of 1-10^0). Spectral observations of DLS is agreed with the results of the analysis of a sphericity coefficient of Voronoi polyhedra constructed for simulated atomic configurations obtained by reverse Monte-Carlo method using experimental structure factors for ball-milled graphite [1].

The work was partially supported by the scientific theme of IMP of NASU № 15/12.

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Spectral investigation of nanodiamonds-onions transitions

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It is well known that carbon onions are generated by nanodiamond (ND) annealing at temperature of 940-1600^{0}C but reverse transitions occur at irradiation of onions by electron or ion beams. A detailed investigation of IR- and Raman spectra (RS) of annealed at 900-2000^{0}C nanodiamonds and carbon onions produced by electrical discharge technology from various hydrocarbon precursors (C_6H_6, C_6H_{12}, $C_{12}H_{26}$ et al) is performed in this work. Nonmonotonic temperature dependences of frequencies, half-widths and peak intensities of D- and G-bands are revealed in the RS of annealed ND with maxima at 1000^{0}C and in an interval of 1500-2000^{0}C. It can be connected with discrete phase transitions in carbon nanostructures, what corroborated by maxima of D_k-bands 1050-1250 cm^{-1} in IR-spectra. Application of different exciting wavelength with λ=514.5, 325 and 257 nm enables ascertaining strong D-band frequency variation in RS of onions at fixed λ. This phenomenon is explained by giant internal self-compression in onions – the interlayer distance decreased to 0.22 nm for interior shells. Corresponding increase of D-bands frequencies (up to 1500 cm^{-1} for λ=257 nm) is accompanied by decreasing ratio of peak intensities ζ=I(D)/I(G).

A quasiliquid diamond-like state of carbon atoms at room temperature is revealed for the first time in cores of onions, connected with the above-mentioned internal self-compression. Its evaluation using 2.8 cm^{-1}/GPa baric shift of 1332cm^{-1} diamond band amounts to 140-250 kbar, what's enough for existence of diamond-like phase. A diamond-graphite phase transition in nanostructures prolongs in temperature interval of ~ 2000^{0}C.

Tuning the optical properties of CdTe quantum dots by the doping and CdS shell growth

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CdTe quantum dots (QDs) have generated tremendous interest due to their unique optical properties that enable effective their applications in optoelectronics, solid-state lighting, solar cells, biomedical fields (in vivo and in vitro imaging) etc.

The formation of the CdTe/CdS core/thick-shell heterostructures with CdS wide band gap semiconductor materials and doping of CdTe QDs are two important techniques that can be used to tune the optical and electronic properties of QDs.

The Hg-doped CdTe QDs. The thioglycolic acid-stabilized CdHgTe NCs were obtained by incorporation of Hg^{2+} ions into already prepared CdTe NCs precursors. Such doping leads to a significant change in the optical properties. We observed bathochromic shift of the PL peaks from 580-590 nm (CdTe QDs) to the near-infrared regions of the spectrum 700-1000 nm as result of Hg-doping on the valence band of the CdTe QDs. Also the absorption maximum is shifted to longer wavelengths and becoming less pronounced. It should be noted that Stokes shift increased from 50 to more than 200 nm.

Type II CdTe/CdS core/shell QDs. The CdTe/CdS core/thick-shell heterostructures were prepared by distillation of solution of CdTe NCs stabilized by thioglycolic acid. The gradual increase of absorption intensity in the short wavelength range was observed. This effect is caused by CdS shell overgrowth due to thioglycolic acid molecules destruction. Moreover, CdTe QDs absorption maximum disappears indicating the type II CdTe/CdS core/shell heterostructure formation after removal of 90% of the solvent. At the same time, the red shift of PL peaks leads to the increase of the Stokes shift due to solvent extraction and solution concentration as results of refluxing of the thioglycolic acid -stabilized CdTe QDs.

Semiconductor nanoparticles as biological labels

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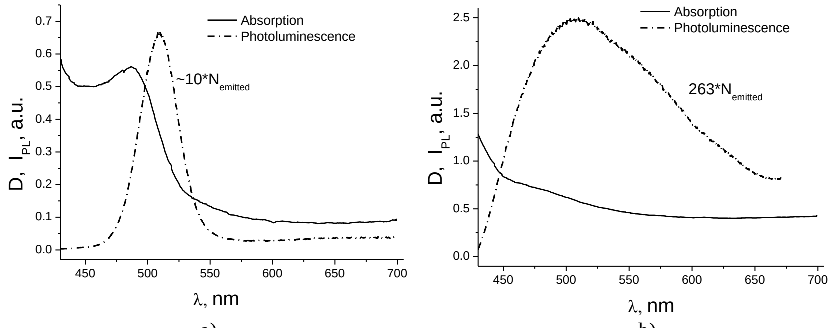
The analysis of biological cells and tissues including precise location of intracellular components labeled with specific fluorophores, their transport characteristics and interactions with other biomolecules can be performed by fluorescence microscopy [1]. Fluorescent semiconductor nanoparticles present a separate class of bright, sensitive, photo-stable and biocompatible semiconductor fluorophores.

Quantum yields and size distribution of different solutions of CdSe semiconductor nanoparticles including grew on our own are measured with the aim to figure out which nanoparticles are better to use as biological labels. The standard (reference) solution is low concentration solution of Rhodamine-6G in ethanol.



a) b)

Fig.1 Photoluminescence and absorption spectra of hexane solution of photo-etched CdSe nanoparticles (a), the same solution without photo-etching (b).

Obtained aqueous solution of CdSe nanoparticles passivated by cysteine has low quantum yield (0.1%) that sets the task of further development of the preparation methodology of nanoparticles in aqueous solution. The most suitable sample for biological labeling is hexane solution of CdSe nanoparticles passivated by decylamine and photoetched by the excitation of argon laser. This sample demonstrates the highest value of quantum yield (64.7%) and the relatively narrow particle size distribution with an average diameter of nanoparticles of 2.1 nm.

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Light-induced resonant heating and vapour generation by water-immersed gold nanoparticles

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The absorption of light by gold nanoparticles in colloidal water solution at the simultaneous excitation of nanoparticles by the continuous-wave laser beam was studied in dependence of the detuning of laser frequency from the surface plasmon resonance. The appreciable blue shift, broadening and increase of intensity of the plasmonic absorption band were observed at approaching of the laser frequency to surface plasmon resonance in Au nanoparticles. The plasmon band broadening is an evidence of laser induced heating of the gold nanoparticles that has an apparent resonant character. The maximal increase in temperature was estimated at 316 K. The sharp blue shift of plasmon band was observed when the temperature exceeded the water boiling point. Such effect is due to formation of the vapor bubbles around the Au nanoparticles occurring at water boiling.

Sensing the temperature influence on plasmonic field of metal nanoparticles by photoluminescence of fullerene C_{60} in layered C_{60}/Au system

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Influence of temperature on the plasmonic field in the temperature range of 78–278 K was studied employing surface plasmon enhanced photoluminescence from the fullerene C_{60} thin film deposited on 2D array of Au nanoparticles. It was experimentally found that temperature dependence of plasmonic enhancement factor of C_{60} luminescence decreases monotonically with the temperature increase. Influence of temperature on plasmonic enhancement factor was found to be considerably stronger when the frequency of surface plasmon absorption band of Au nanoparticles and the frequency of fullerene luminescence band are in resonance. Electron-phonon scattering and thermal expansion of Au nanoparticles were considered as two competing physical mechanisms of the temperature dependence of plasmonic field magnitude. The calculations revealed significant prevalence of the electron-phonon scattering. The temperature induced increase in the scattering rate leads to higher plasmon damping that causes the decrease in the magnitude of plasmonic field.

The amplification of spontaneous emission and non-elastic scattering process in the nanocomposites based on synthetic opals

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Synthetic opals (SO) are the globular 3D photonic crystals and offer great opportunities for studying the effects of spontaneous emission amplification, low-threshold lasing, light localization and etc.

The aim of this work is to study experimentally the physical reasons for the influence of structural defects on spontaneous emission and non-elastic scattering process of the nanocomposites based on the synthetic opals.

The fluorescence spectra of the opals infiltrated with Rhodamine 6G (R6G) have been measured in the ‘reflection’ geometry under absolutely identical conditions. Three samples with different ordering degrees defined by introduced ordering coefficient η_{order} have been used. The concentration of R6G molecules in the infiltrated solution for all the samples has been the same. The ratio I_{SO}/I_0 of the integral intensity for R6G in the SO to the integral fluorescence intensity of R6G–ethanol solution in an optical cell is the criterion indicating to amplification of spontaneous emission in the SO. The fluorescence spectra reveal an increase in the integral luminescence intensity with increasing amount of structural defects in the opals. This increase in the intensity correlates with the increase seen for the ordering coefficient η_{order} and, consequently, the increase of ‘slow’ exciting photons with a diffusive distribution character.

We have also measured the Raman spectra for the control sample with the $Bi_{12}SiO_{20}$ powder and SO filled by $Bi_{12}SiO_{20}$. The comparative analysis of these spectra showed a significant (over 3 times) amplification of the Raman lines integral intensity. A mismatch of the Raman spectral range and the spectral position of the photonic stop-band in our samples suggest that the amplification in our case is rather due to the multiple scattering of excited photons.

Energy Spectrum on Traps in Yttria-Stabilized ZrO_2

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We present the results of studying the thermostimulated luminescence of Yttria-Stabilized ZrO_2 (YSZ) with different amount of Y_2O_3. This material has a wide spectrum of applications, such as the oxygen sensor, the electrolyte in fuel cells etc due to relatively high ion conductivity[1]. Studies of nanocrystalline YSZ in order to move to a more optimal technology for fabrication and improvement of its characteristics [2] remain steel perspective.

A characteristic feature of the bands of the YSZ thermoluminescence is a wide almost structureless band in the range of 85 - 200 K with a maximum at ~ 110 K. Half-width of band increases with the concentration of yttrium oxide and new high-temperature components appear. We found that the band consists of 2-3 highly overlapped peaks, that correspond to release carriers from energy levels of traps (activation of carriers).

The analysis of increase of the intensity of thermo-luminescence from the temperature allowed to obtain the energy of traps. We used the method of partial thermal bleaching of the glow [3]. The calculated values of activation energy of traps in YSZ (for samples with different percentage of Y_2O_3) are within 0.15 - 0.5 eV. In general, the results show a monotonic increase of the activation energy, this is due, in particular, the significant overlapping of thermoluminescence bands. However, there is barely expressed a series of monoenergy values corresponding to activation energy certain traps.

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9

Surface

Spectral and luminescence properties of the hybrid film as result of intramolecular interaction and mesoscopic ordering of self-assembled dye in hybrid film

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Dependence of the spectral-luminescent properties of guest molecules from their electronic and chemical structure had been studied before, while for most practical applications, condensed matter is necessary. Fluctuations of the intermolecular interaction energy lead to the experimentally observed broadening of the electronic level's energy of organic dye and alternate their fluorescent properties. We show the possibility to fabricate of the mesoscopically organized hybrid films doped with dyes are prepared for use as photochromic materials, optoelectronic devices. Unusually effect of the impact of dye concentration on the fluorescence affectivity was established. The interaction of the dye molecules and the inorganic matrix leads to significant changes of the intensities of the absorption and photoluminescence. The further increase of the concentration leads to mesoscopic ordering, beyond of intermolecular interactions and percolation treshhold toward oblique aggregates and increasing of the fluorescence intensity due to the confinement of the dye molecules involved in the intermolecular and intramolecular interactions within the film structure. For such a hybrid, method of stationary and time-resolved luminescence was found that organic-inorganic films characterized by the formation of dimers with a fast component of exciton, which is a prerequisite for the use of composite films as photonic coatings [1].

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Obtaining and physical properties mono - and multilayers silver nanostructures

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By high-resolution tunneling microscopy there were investigated silver nanostructures on the Si (111) surface It has been revealed that silver on the surface of silicon can form nanostructures consisting of atomic planes. Metallic nanostructure neoplasms can take the shape of regular hexagons. For these structures, minimum height of the step growth varies in the range of 0.23 nm. Specific peculiarities of the nanorelief transformation with temperature increasing of the sample are detected as a result of horizontal displacement due to surface drift. The possibility of preserving of the Si (111) 7x7 structure is presented.

With increasing sample temperature to 300 ºC was fixed decrease in the number up to three metal monolayers (Fig.1a). In this case figures are absent of regular shape, the height of growth of nanostructures remains, and silver completely covers the surface of silicon. During slow increase in temperature of the sample to 400 °C (Fig.1b) occurs silver desorption, and recovery of surface Si (111) 7x7. This fact testifies to the allegation that the connection between the substrate and the deposited metal weak. Silver in the process of deposition at room temperature does not penetrate the Si.

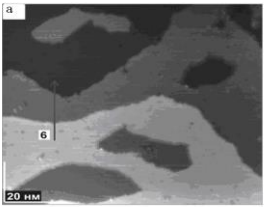

Fig. 1a) STM imaging Ag deposited on Si (111) at T=300 °C (100x100 nm^2).

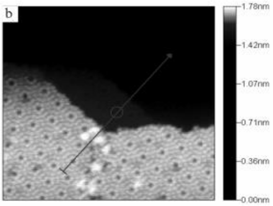

Fig. 1b) STM imaging of the surface of the silicon single crystal with the structure of 7x7 after heating to a temperature of 400 °C.

So after heating the sample for 2 minutes at a temperature T = 400 °C occurs reproduction 7x7 reconstructed surface of a single crystal, which indicates that deposition silver not leading to destruction of the surface that is possible conservation structure surface Si (111) 7x7.

Spectroscopy of amorphous carbon on glass substrate and amorphous carbon on thin copper layer

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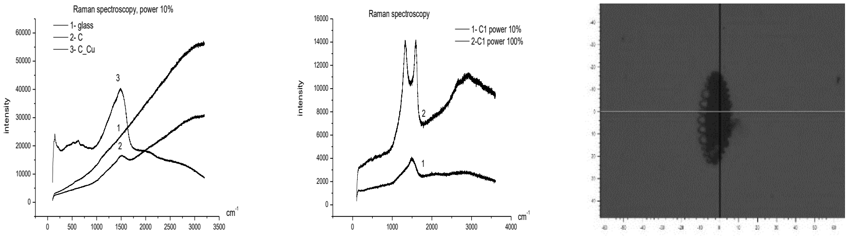
Thin films of copper and amorphous carbon (α–C) on glass substrate were deposited using the vacuum deposition method.

Raman spectroscopy as an informative non-destructive method plays an important role in studying of carbon materials (α–C) structure. In the monophonon Raman spectrum of graphite perfect single crystals only one known narrow line *D* at 1581 cm^{-1} is observed. In α–C usually two very wide overlapping bands with peaks at 1540–1560 and 1340–1370 cm^{-1} are seen – so-called bands *D* and *G*. The first of them corresponds to the mode associated with symmetric stretching-pressing vibrations of sp^2-bonds, the second corresponds to defects in the graphite structure. Research has shown that the position of both *D* and *G* bands of α–C depends on the activating radiation wavelength. The peaks position, width and relative intensity of the bands depend on the film preparation technological conditions. Figure 1 shows a Raman spectrum of glass substrates (*1*), α–C film deposited on the glass (*2*), α–C film deposited on the copper underlayer (*3*). As seen, the intensity of the composite α–C:Cu Raman spectrum is the highest. This interaction leads to a change of the Raman spectrum shape when the activating radiation with high intensity is used. Figure 1 *b* shows the Raman spectrum shape change depending on the intensity of the activating radiation. Figure 1 *c* shows the change in color and shape of the α–C exposure spot as a result of the activating radiation effect. This can be explained by the plasmon interactions between the metal layer and α–C layer, as well as phonons mean free path increase.



a *b* *c*

Raman spectroscopy of copper thin films

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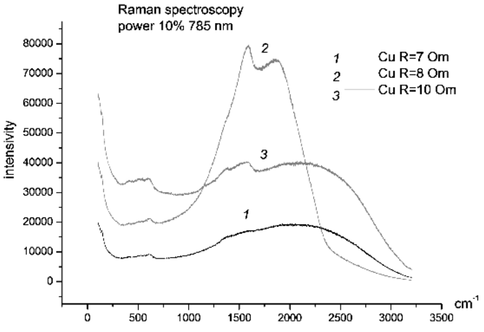
Thin metal films are objects with a very wide range of physical properties that significantly extends their practical application. Thin copper films on glass substrates were obtained using the vacuum deposition method during the current research. Thin films absorption and electrical resistivity (in the range from 5 Ohm to 10 MOhm) were controlled in different deposition conditions. It was theoretically shown in work [1] that in metal thin films, surrounded by dielectric, can occur plasmons with mean free path substantially exceeding the mean free path of plasmons existing at the metal-dielectric border. The properties of the surface plasmons essentially depend on thin films cluster structure with such significant parameter as ratio of cluster size to the size of gap between the clusters. The figure shows the Raman spectrum of copper films with an electrical resistance 7, 8, 10 Ohm, obtained in different conditions of vacuum deposition P7>P8>P10. It shows that film with the highest intensity of Raman scattering has an electrical resistance of 8 Ohm. This allows concluding that there are the largest local fields in this film, determined by localized surface plasmons. Such films are of greatest interest. The measurements of absorption spectra in the visible range show that there is an absorption peak at 570 nm, which indicates the existence of copper oxide in the obtained films. This is confirmed by the electrical resistance of copper films increase occurred after air is admitted into evaporation chamber, and also by the Raman peak in the range of 560 cm^{-1}. Copper oxides are characterized by charge states capability, which is essential for plasmonic properties of thin films.



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Tunneling spectroscopy of $Fe_{82}Si_4B_{14}$ amorphous alloy

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Using methods of high-vacuum tunneling spectroscopy at atomic resolution electronic structure of $Fe_{82}Si_4B_{14}$ amorphous metal alloy have been investigated. STS allows obtaining the I-V curves of the samples for electrical features explanation. Investigations were carried out for the same sample with a gradual temperature increase from 300 to 700 *°C*. Differential dependence *dI/dV* have allowed us to determine the electronic bandgap and occupied electronic states at the surface of the amorphous $Fe_{82}Si_4B_{14}$ metal alloy for each temperature range. Due to heterogeneity of the surface at different points a variety of electronic properties has been observed. Unique feature such as change of the bandgap in surface electronic spectra until the temperature increases, that may be due to the segregation of light elements on a surface such as silicon and boron, was seen. On tunneling spectra can be clearly seen the occupied states in the valence band which can be strictly tied to 3d Fe sheath. These effects are observed only on the surface and do not lead to significant changes in the conductivity of $Fe_{82}Si_4B_{14}$ amorphous metal alloy as a whole.

SERS-active substrate on base gold nanoparticles or nanocrystals-nanoprisms

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During investigation of the surface enhanced Raman scattering (SERS) of single molecules as substrates usually use the roughness surface of the noble metal layer such as Ag, Au, and Cu or the water solution of nanoparticles (NPs) based on these metals. The enhancement factor strongly depends on size and shape of NPs and their concentration in the suspension.

Here, we report of the results our investigation of the Raman spectra for polysaccharides (PS) macromoleculs of the microalga *Chlorella vulgaris* LARG-3 which are adsorbed on the surface of Au NPs and nanocrystals.

Spherical Au NPs were synthesised using Devis' method [1]. In order to form the adsorption layer on the surface of Au NPs we added water solution of the PS (C_{PS}=40 mg/dm^3). Gold nanoprisms of the different shape such as triangular and hexagonal with length of 0.2÷10 μm and thickness 20÷40 nm were obtained by reduction $AuCl_4^-$ ions (precursor $HAuCl_4$) in the water PS solution [2].

The substrates for studying Raman spectra have been formed from Au NPs or nanoprisms. For this purpose, the drop suspension of Au nano-particles/-prisms with adsorbed PS layer was deposited on the surface of freshly prepared mica and then dried up at room temperature. The Raman spectrum received from PS after drying of a drop (20 μl) pure water solution PS (C_{PS}=40 mg/dm^3) on a mica surface was control. Raman spectra were recorded using a Renishaw 1000UV spectrometer with the excitation wavelengths of 632.8nm, power 1 mW and diameter of the focusing beam 1-2 μm.

We compared the intensity of main Raman lines for control PS sample and for PS molecules on surface of Au nanospheres and revealed a small enhancement for vibration line (1598 cm^{-1}) of the carboxyl group. Interestingly, that in the Raman spectra of PS adsorbed on top of Au nanoprisms the feature at 618 cm^{-1} disappeared (which is attributed to the stretching vibration mode of COOH) and peak at 1598 cm^{-1} splitted at two 1593 cm^{-1} and 1521 cm^{-1}. The strongest enhancement was found for peak at 1521 cm^{-1} with enhancement factor about of 20. It was shown that the SERS for active Raman lines essentially increases when the focusing laser beam located exactly on top of Au nanoprisms. The results showed that the SERS increases with the change in nanoparticles' shape from nanospheres to nanoprisms and last nanostructures can be used in future as Raman active substrates.

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Optical properties of transition layer in system “oxide’s thin film – bulk metal”

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The optical properties of aluminium oxide’s thin film – bulk metal system were modeled. Two-layer model: aluminium oxide – interlayer – bulk metal was used in the work.

Spreading light through these system was representing in matrix form. The refractive index of transition layer n_2^* was deemed as a complex value $n_2^* = n_2 + i k_2$, where n_2 and k_2 - the index of refraction and absorption of the transition layer, respectively. The reflection coefficient’s dispersion R(λ) in wide spectrum range (λ = 0.2 – 1.2 nm) was calculated for dielectric-transition layer-substrate system using two layer model. The aluminium oxide layer was applied with different thickness (200 -300 nm). Oxide films deposited on a specially prepared surface of metal laser mirrors from solid aluminum and copper.

The results obtained from the use of single and dual-layer models were compared and determined that the transition layer was formed. The characteristics of this layer were determined by comparing the experimental and calculated data in whole range of reflection coefficient’s dispersion measurements and in some areas of the spectrum.

Optical and geometric characteristics of oxide-metal system’s transition layer were determined. It was determined a good agreement between calculated and measured data.

Structure, morphology and photoluminescence of vacuum deposited rubrene thin layers

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Among organic semiconductors, rubrene ($C_{42}H_{28}$, 5,6,11,12-tetraphenyltetracene, Rub) is extensively studied in recent years since it exhibits interesting physical properties such as very high charge carrier mobilities in organic field effect transistors at room temperature. Rub is used as a laser dye and as a fluorescent dopant in many other OLEDs to improve characteristics such as lifetime, stability, color and brightness. However, there are controversies as to the Rub degradation both in the bulk state and thin layers, so better understanding of these phenomena is crucial for improving the performance of organic devices. In this work we present the results on complex studies of the structure, morphology and photoluminescence (PL) properties of Rub layers deposited on freshly cleaved KBr and atomically smooth Au(111) surfaces by vacuum thermal evaporation. Thickness of the Rub layers was controlled by digital quartz balance monitor, and varied from 35 to 120 nm. FTIR absorption spectra of the obtained samples were measured at room temperature (Bruker IFS-88, 2cm^{-1} resolution, 64 scans) and confirm stable vacuum deposition behaviour of Rub. No evidence for the formation of crystalline grains was found, which indicates amorphous structure of the as-deposited Rub layers on KBr substrates. The morphology of the first near-surface layers of Rub deposited on atomically flat Au(111) surface was investigated with STM method, which reveals molecular rows preferentially oriented along (112) direction of the substrate. Reproducible STM-images were recorded at scanning parameters: I_t=100÷170 pA, U_t=800 mV. Increasing of bias up to 1V led to instability in tunneling gap due to polarization and desorption of Rub molecules. STM current-voltage spectra did not reveal asymmetry. From the changes with time in the peaks position and intensity of room-temperature PL spectra of the films, the Rub degradation kinetics is analyzed depending on the film deposition conditions.

Influence of Au(111) surface functionalization by n-alcanethiols on its wetting properties

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Knowledge of the wetting behavior of solvents on surfaces is notably important in the interest of basic physics, but also for many industrial processes and applications such as cleaning, coating etc. Self-assembled monolayers (SAM) film have provided new and easier ways to control the physical and chemical properties of surfaces. In this context, thiols molecules (alcanethiols) are perspective for study main principles of creating hydrophilic/hydrophobic surfaces.

Besides, using Au(111) as a substrate reveals an unique opportunity to study the dependence of the surface wetting properties from its functionalization by scannig tunneling microscopy (STM).

In current research, 11-Mercaptoundecanoicacid [MUA], 11-Mercaptoundecanol [MU], 1,4-Butanedithiol [1,4-buta], 1,9-Nonanedithiol [1,9-nona], 1-Dodecanethiol [1-Ddc] SAMs are studied. Au(111) were as a substrate.

It is shown that the presence of hydrophilic groups on the surface increases wettability.The study demonstrates the influence of length of molecules alkyl chain on hydrophilicity. It is founded, increasing of aliphatic chain leads to increasing hydrophobicity. It is suggested, that the observed effect is due to peculiarities of self-assembling of molecules.STM-investigations of n-alcanthiols monolayers approved hypothesis of the influence of functionalization degree of surface on its wetting properties.

STM allowed to eastablish stucture of alcanethiols SAM in nanometric scale. It is detected typical for thiols “leopard-like structure”. STM-images are revealed stuctures with well-defined molecular rows. Rows Orientation coincides with the main crystallographic directions Au (111). STM images with molecular resolution for MU are founded hexagonal packaging bright spots. Since the distance between adjacent spots is corresponding to the diameter of the functional group -OH, we attribute them to individual molecules thiol MU. [1,4-buta], [1,9-nona], [1-Ddc] SAMs have a similar packing. For them STM-images were obtained by scanning with relevant parameters.

Ellipsometric properties of thin Ti films considering roughness and inhomogeneity of the transition layer at excitation of surface polaritons

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In the paper [1] it was shown that ellipsometric parameters of thin semi-transparent Ti films without excitation of surface polaritons are well described with three-layer film model where the central layer has optical constants of massive Ti and the upper and lower layers respectively have optical constants of titanium oxides. The same has been shown in the paper [2] considering thin semi-transparent Mo films. But in the paper [3] were conducted ellipsometric research of thin Mo films at excitation of surface polaritons. Herewith the experimentally measured and calculated on a three-layer film model ellipsometric parameters Ψ-azimuth of restored linear polarization and Δ-phase shift between p-and s-components of the reflected wave had only qualitative match (experimental course of angular dependences of these parameters and course calculated on a three-layer film model were identical). Quantitative match was poor. The latter was explained by the fact that all three papers considered the interface between layers as perfectly flat, but actually they are rough and inhomogeneous. In standard ellipsometry where the wavelength is much larger than roughness size it feels poorly. At the same time polaritons are moving on the surface and feel all the roughness and inhomogeneity much stronger. Therefore, in this paper it was decided to use a fourth layer located between the substrate and Ti film, describing the inhomogeneity and roughness of the substrate surface. Experimental measurement of ellipsometric parameters and calculations on computer have shown that four-layers film model has a qualitative and quantitative match between experimentally measured and calculated angular dependence of ellipsometric parameters. Analysis of optical constants of the transition layer between the glass substrate and Ti film showed that it consists of glass granules, intervals between which are filled with Ti oxide.

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Ellipsometric study of CdTe films on BaF_2

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Spectral (314 – 579 nm) ellipsometric study was conducted for CdTe films grown on the monocrystalline BaF_2 substrates by the vacuum “hot-wall” epitaxy method at different temperature of the substrates (100 – 300 ºC).

The inner structure of the film was defined. It could be presented by several layers with different thicknesses and optical constants.

The layer adjacent to the BaF_2 substrate is a layer of bulk CdTe with the thickness up to 300 nm. The upper layer is an interlayer with thickness of about 35 nm and optical constants that corresponds to the mixture of CdTe and its oxide with volume fraction 0.5.

The outer layer is a layer of strongly distended CdTe with thickness up to 30 nm. Optical parameters of the layer and its composition correlate with substrate temperature correspondingly. Specifically indexes of refraction and extinction increases with temperature rise, volume fraction of the films’ matter in the outer layer increases correspondingly.

Temperature dependence of ELC layer thickness

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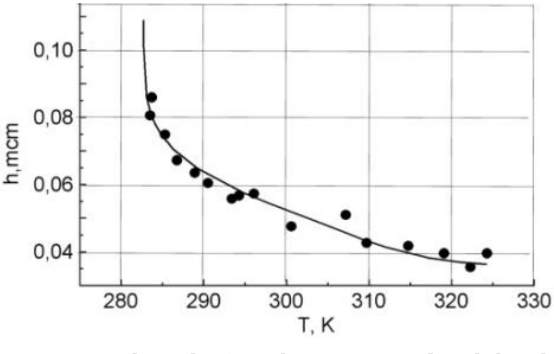
In our report some properties of metastable orientationally ordered state of wall adjacent liquid layer (so called epitropic liquid crystal – ELC) are discussed. Heating of ELC layer leads to decreasing of its equilibrium thickness. We suggest a quantitative theoretical explanation of this phenomenon.

According to a model of ELC formation [1] it is assumed that orientational ordering is induced in ultrathin wall adjacent layer by a solid substrate. Intermolecular interaction causes to a relay race mechanism of orientational ordering transfer into the bulk liquid. In this model the thickness dependence of order parameter S(z) is calculated as a solution of differential equation. This solution depends on 2 parameters, which in turn are the coefficients of expansion of intermolecular interaction potential on the Legendre polynomials. These coefficients depend on the temperature and liquid density and their values determine the possibility of 3 types of solutions which correspond to nematic, isotropic and ELC phase. The ELC equilibrium thickness is estimated as the distance between the wall and inflection point of calculated curve. Its value is determined by the second coefficient of above mentioned expansion, which in turn depends on the temperature.



Simultaneously almost similar results were obtained in the framework of two-componential model [2], which assumes the coexistence of dimers and monomers in liquid layer near the surface of the solid substrate. The figure illustrates the relatively good agreement of calculated dependence and experimental results (nitrobenzene near lyophilized quartz substrate).

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Surface doping effect on optical absorption and luminescence of TiO_2.

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We have investigated the surface doping effect by Cr cations on the optical absorption and laser-induced luminescence of rutile and anatase TiO_2 at room temperature. Nanocrystalline anatase (*A*) and rutile (*R*) TiO_2 were synthesized by the thermal hydrolysis and then were surface doped with Cr ions by adsorption from $CrCl_3$ solutions. The samples were characterized by X-ray diffraction, X-ray fluorescence, Raman spectroscopy, optical absorption and photoluminescence (PL) methods. It is found that the PL emission and optical absorption near the band gap edge occur with the same electronic transitions in TiO_2. The influence of surface doping effect on the rutile TiO_2 optical absorption and PL spectra is discussed.

For the first time, excitonic and band-to-band luminescence of nanocrystalline *R*/Cr and *A*/Cr TiO_2 is observed using a high-intensity N_2 laser excitation at room temperature. A detailed analysis of the *R*/Cr and *A*/Cr TiO_2 absorption and PL emission spectra is carried out. It is shown that the Cr^{3+} doping leads to the blue and red shifts of the PL peaks in *A*/Cr TiO_2 due to the Burstein-Moss and band tailing effects, respectively. The Auger type non-radiative recombination in *R*/Cr TiO_2 quenches the PL emission intensity. For anatase samples at low concentrations of Cr ions (0.5 at. %) the PL emission increases compared to the undoped *A* TiO_2 due to the formation of additional radiative recombination centers. At higher contents of Cr (1.0 at. %), the PL intensity decreases due to the concentration quenching effect.

Raman spectroscopy of two-dimensional materials based on amorphous carbon

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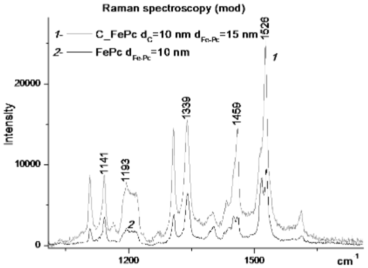
In the course of conducted research using the method of vacuum deposition on glass substrates thin films of amorphous carbon (α–C) with films of phthalocyanine (FePc) class organic molecules were obtained.

The Raman spectroscopy showed an increase in oscillation modes for films FePc with thickness d=15 nm and (α–C) with d = 10 nm. Thin films FePc show up increased oscillation modes and have higher absorption at 300 nm and 560 nm bands. This can be explained by two mechanisms affecting the intensity of the Raman spectrum, causing the intensity of local magnetic fields rise in the system (α–C, FePc) structure (electromagnetic mechanism) or chemical interaction between α–C and FePc. The second mechanism usually affects less than the electromagnetic one [1]. The figure shows the Raman spectrum with background compensation for system (α–C, FePc). The interpretation of the Raman spectrum peaks are given in the table, as in [2].



	cm^{-1}	Mode description
A_{1g}	1141	H–C–C
	1193	H–C–C, C–C benzene
A_{2g}	1339	H–C–C, C–N_α
B_{2g}	1459	C–N_α,C–C pyrrole, H–C–C
B_{1g}	1526	C_β–C_β, H–C–C

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Laser-induced quasi-periodic metal structures for efficient excitation of surface plasmons

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Formation of laser-induced periodic structures on metal surface are an interesting subject of theoretical and experimental investigations. Metallic nanostructures has advantages due to their capability of supporting collective electron oscillations or plasmons, which are involving in a number of effects including spectrally tunable absorption and scattering, local enhancement and strong confinement of electromagnetic field at length scales much smaller than the optical diffraction limit, etc. Such unique properties can provide many important applications such as surface enhanced Raman spectroscopy (SERS), plasmonic emitters, active plasmonic devices, biosensors, etc.

Micro- and nanostructures on silver, copper and aluminium surfaces were formed by treating the surface with the emission of high-power Ti:sapphire femtosecond laser. Surface peculiarities and parameters of these laser-induced periodic structures have been analysed by the methods of atomic-force microscopy (AFM) and investigation of the light-scattering indicatrices. In particular, obtained structures have several different periods and nanogranular fine structure. Possible mechanisms of formation of such structures have been considered. Conditions of the excitation of surface plasmon polaritons on the structured metal surfaces have been also studied by the measurements of the specular reflectance spectra.

The effect of surface enhancement of Raman scattering of Rhodamine 6G (Rh6G) dye on obtained laser-induced silver nanostructures has been revealed, indicating a promising application of laser-structured surfaces for gain of some linear and non-linear optical processes. For some vibrations of Rh6G molecules the maximal enhancement factor of 10 was obtained.

Vibrational spectra of ZnO:Ir thin films

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ZnO:Ir thin films on Si and Ti substrates were deposited by reactive DC magnetron sputtering at room and 300°C temperature. Properties of films were investigated as a function of iridium concentration in the films by XRD, Raman and FTIR techniques.

XRD measurements show that light doped ZnO thin films with Ir are oriented in the c-axis direction. Frequency of LO and TO vibrational modes shifts from 570 cm^{-1} and 410 cm^{-1} for undoped ZnO to 635 cm^{-1} and 465 cm^{-1} for 20at% Ir doped ZnO respectively. Raman spectra of 20at% Ir doped ZnO show new features with strong band at 720 cm^{-1}.

Ab initio calculations were used to model vibrational frequencies.

Raman spectra of SiC/TiO_2 structures

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High thermal stability, large values of the dielectric constants and the relative simplicity of the technological processes of growing of some rare earth oxide films make these films promising for the insulating layers in microelectronic circuits. In particular, the actual problem for the high-temperature electronics based on silicon carbide is to develop the stable high-quality dielectric layers, including ones on the basis of oxide films of titanium, erbium and gadolinium. Despite the wide range of technical possibilities of producing of metal oxide films (from the anodic to oxidation in air or in an oxygen atmosphere, in water and in water vapour, in carbon dioxide or in various other gas mixtures), the search of well-controlled, rapid methods of forming of metal oxide films with reproducible parameters is still continued.

The metal oxide films have been obtained by oxidation of thin Ti metal films using rapid thermal annealing (RTA) at T = 623K for 1, 3 and 5 s. The thicknesses of oxide layers defined by multi-monochromatic ellipsometry are 34-65 nm for the titanium oxide films. The study of Raman spectra of SiC/TiO_2 structure after the RTA revealed that in the range of 300-600 cm^{-1} in addition to the vibration bands specific to 6H-SiC there are bands that indicate the formation of a titanium oxide film on the surface of SiC, which correlates with Auger spectroscopy data. Thus, the analysis of the experimental data concerning the producing of Ti oxide layers on the surface of SiC showed that the RTA method allow to form oxide film with a thickness of less than 100 nm.

Deposition and optical constants of Cu_6PS_5Br thin film

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Cu_6PS_5Br crystal belongs to argyrodite family and is well known as a superionic conductor. They possess high ionic conductivity and low activation energy what makes it promising for applications as an electrochemical energy source. The efficient ion transport is explained by the specific crystalline structure which facilitates fast ion transport.

Cu_6PS_5Br films were deposited on c-cut sapphire substrates at room temperature by means of high target utilisation sputtering from target in radiofrequency Ar discharges. The plasma source power density was fixed at 2000 W yielding a deposition rate of approximately 1.5 nm/min. Target pulsed DC power was fixed at 70 W. All depositions were carried out at floating plasma potential. The base pressure in the chamber was below 7×10^{-4} Pa and the total working gas pressure during deposition was kept at 0.65 Pa. Structural studies were carried out using X-ray diffraction and SEM techniques. The diffraction pattern shows the film to be amorphous with crystalline inclusions.

The dispersion dependences of the refractive index and absorption index for the Cu_6PS_5Br thin film were obtained from the spectral ellipsometer measurements in spectral range 0.4-1.0 μm. Thus, the refractive index at $\lambda = 1$ μm for thin film equals 2.362 while for crystal it equals 2.582. The slight dispersion of the refractive index is observed in the transparency region while it increases when approaching to the optical absorption edge region. The optical absorption edge spectrum as well as the dispersion dependence of refractive index of Cu_6PS_5Br thin film were analysed.

Spectroscopic investigation of dicarboxylic azelaic acid adsorption by KIT-6 mesoporous silica

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Dicarboxylic acids are organic compounds that contain two functional carboxylic acid (–COOH) groups. Industrially, they are important in production of polyester, polyols, polyamides, and nylon and as a precursor to active pharmaceutical ingredients and additives. Dicarboxylic acids are important water-soluble components of atmospheric aerosols. Bactericidal antiseptic properties of carboxylic acids are widely used in medicine and food industry. Dicarboxylic acids specific properties depend on the mutual influence of the two carboxyl groups.

In this report, the adsorption of azelaic acid by KIT-6 mesoporous silica is investigated using Fourier transform infrared (FTIR) spectroscopy and differential scanning calorimetry (DSC). With FTIR analysis, it is shown that azelaic acid carboxyl groups adsorb predominantly on outer-sphere KIT-6 surface. No crystallization of the adsorbed acid species is found using DSC analysis. The adsorption types, inner- or outer-sphere, depend on the azelaic acid species, pH, and solvent conditions, and different conformations and aggregations of the adsorbed acid are discussed to establish a more detailed surface complexation model.

10

Theory

Current through two quantum dots in a magnetic field

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The aim is to study the processes of electron transport in nanosystems. The system, which is investigated, consisting of two quantum dots connected with each other and attached to electrodes. Quantum dots are placed in a constant magnetic field. Single level quantum dot is quasi-zero-dimensional model of impurity atoms, which is formed Anderson`s electron localization. The main research method is the method of equations of motion for two-time Green's functions in the Keldysh formalism. The calculation of current and differential voltage is performed in approaching of the general area. Numerical calculations performed for the stationary case. This research presents theoretical and practical interest and is a part of the problems concerning development of modern and future electronic nanodevices and quantum computation (applying a small voltage to control the flow of electrons through the quantum dot and their polarization).

Elementary wave packets decomposition – new spectroscopy technique

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As usually Spectroscopy investigation means decomposition of the electromagnetic wave or physical process into orthonormalized serie of harminic functions. These functions are rather simple one, therefore Fourier spectroscopy (FS) has found a wide utility in Physics and Engineering. The grave practical disadvantage of FS is its nonphysical properties of basic functions. The second silent assumption in Optics is 'slowly varying envelope aproximation" or 'narrowband signals". However for superwideband pulses this aproximation no longer hold ,for example, in Femtosecond Optics.

In 2009 [1] we proposed method of describing electromagnetic pulses as ortho- normalized series without restriction on their durations. The proposed series was used for analysis and synthesis of electromagnetic signals [2]. Another problem concerns Physical Optics that consider electromagnetic waves interactions with the matter. We proposed to use EWP-modes aproximation for optical wave propagation description [3]. Then the dielectric properties of substence could be presented as the matrix, which elements represent time dependences of EWP-intermodes conversion.

So one can say that EWP-decomposition can be used in nonstationary Optics for laser pulses analysis and synthesis and characterizing of dielectric properties of matter.

We have developed model of EWP-Spectrometer with the correlator circuit design. It contains a generator of basic elementary wave packets functions, multiplier and integer unit. Technical base for the engineering was ATmega Microcontroler family.

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Combinatorial mechanism of broadening of the O-H stretching bands in hydrogen bonded molecular clusters

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A new broadening mechanism for collective vibration bands is supposed. It allows explaining the experimentally observed increasing of bandwidths of the O-H stretching vibrations upon increasing the number of molecules forming a molecular cluster. In the zero-order approach, to calculate halfwidths of absorption bands of the stretching vibrations of hydroxyl groups in clusters containing several molecules it is enough to know only the halfwidth of the band of the stretching vibration of a donor O-H group in a dimer ($\Delta\tilde{\nu}_1$), wavenumbers of the maximums of the bands in hand ($\tilde{\nu}_1;\tilde{\nu}_Z$) and the number of hydrogen bonds (Z):

$$\Delta\tilde{\nu}_Z = \frac{\tilde{\nu}_Z\left(1-(1-2\pi\frac{\Delta\tilde{\nu}_1}{\tilde{\nu}_1})^Z\right)}{2\pi};$$

It is shown that there is a good agreement between the calculated and presented in literature data on the values of the absorption bands halfwidths for propanol and methanol clusters (see Table 1).

Table 1. The halfwidths of the O-H stretching bands in propanol clusters calculated in the context of the combinatorial broadening model and the corresponding experimental values (with their error in parentheses).

Number of H-bonds in the cluster (Z)	Calculated values $\Delta\tilde{\nu}_Z$ (cm^{-1})	Experimental values $\Delta\tilde{\nu}_Z$ (cm^{-1}) [1]	Experimental values $\tilde{\nu}_Z$ (cm^{-1}) [1]
1	47	55(3)	3521
2	88.1	83(5)	3444
3	124.2	118(7)	3376
4	153.6	145(4)	3264

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Optical trapping of atoms and molecules by bichromatic field

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One of the most popular laboratory equipment in low-temperature atomic physics is the magneto-optical trap [1], which based on the atom's interaction with laser light and the magnetic field. An alternative optical trap, which does no use magnetic field, proposed in [2], is based on the sequences of the counter-propagating laser pulses. Recently the authors of [3] showed that such a trap could also cool the atoms, if the parameters of the atom-field interaction are properly chosen. In the report, we come back to the old proposition [4] of trapping atoms by bichromatic field of two standing waves. As it was emphasized in [4], the physical background of the light pressure force in these waves is close to one in the field of the sequences of counter-propagating laser pulses, so we can expect trapping and cooling of atoms by bichromatic field too. An example of numerical simulation of a sodium atom's motion depicted in Fig. 1 confirms our expectations. This trap can also trap the molecules with almost diagonal Franc-Condon factors array.

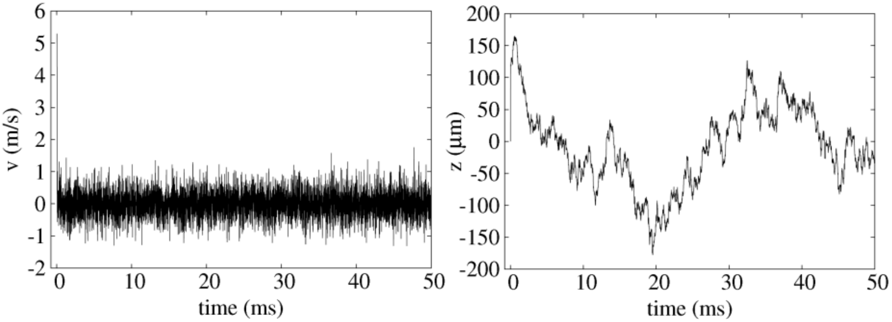

Fig. 1. Dependence of Na atom velocity and coordinate on time. Rabi frequency of each wave is 100 MHz, difference of wave frequency is 200 MHz, red detuning of the average frequency from the atomic transition frequency equals 5 MHz.

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Wave propagation in an ellipse: A concentration energy effect

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The unique properties of an ellipse are widely used in different fields of science and technology: optics, spectrum analysis, solar power [2], acoustics, medicine etc. In particular, the focal property of an ellipse is applied in Raman scattering investigations, where elliptical mirrors are used for focusing light [2]. It should be noted also another interesting phenomenon called “quantum mirage” directly related to the specific properties of an ellipse [3].

In this paper, the redistribution of wave energy, which is excited in the focus along wavefront after certain number of reflections from the ellipse wall, is discussed. We assume that the propagation medium is ideal, without dissipation of wave energy. Distances passed by the element of the wavefront after overpassing the focus and angles between the big semiaxis and trajectory of particle path are given. It is analytically shown the motion of the element of the wavefront after some number of reflections from ellipse walls takes place only along big semiaxis. Carried out geometrical scheme and process of the redistribution of the energy in an ellipse modeling by Excel show that wavefront after several reflections from the border of an ellipse cease to be uniform and energy of wave is concentrated at sites of big semiaxis only. The wavefront originally having the form of concentric circles is transformated into a localized impulse. Thereby, in the frame of the given model, it is shown that in an ellipse the effective collecting and concentrating of energy can take place.

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Radio-frequency emission of cylindrical macroparticles in heterogeneous combusion plasma

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A new statistical approach to the modeling of radio-frequency (RF) emission of macroparticles with cylindrical shape in combustion plasma of solid fuels is proposed. The main attention is focused on the translational and rotational constituents of inharmonic vibration modes for cylindrical macro particles. The chaotic motion of them is produced on the ensemble of momentary individual electro neutrality cells (see [1, 3], Fig.1., Fig.2.). However, taking into account of rotation all degrees of freedom changes the spectrum into radiation condensed phase.

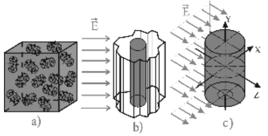

Fig.1. Statistical averaging of the instantaneous cylindrical cells of electroneutrality heterogeneous plasma (HP).

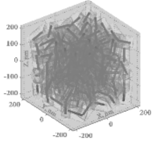

Fig.2. Translational and rotational movement of cylindrical particles in the HP.

Distortions of the averaged shape of cells arising due to translational and rotational displacement of particles are determined by changes correlation energy. Spectra and intensivities of different modes art found in the approximation of chaotic phases. The computer simulation of the radio-emission for the zirconium oxide and aluminum oxide is carried out manifestation of the specific contribution in integral radiation is analyzed (see Fig.3., Fig.4.).

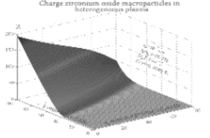

Fig.3. Electric charging of particles of zirconium oxide in the plasma.

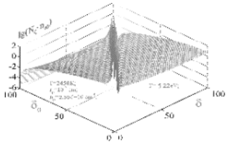

Fig.4. The power density of the radio emission electronic components HP

The tele- diagnostic of the heterogeneous plasma with all mentioned processes is considered. Contributions in RF- emission stochastic rotation macro particles is studied separately.

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Physical evidences "for" and "against" H-bonds

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H-bond is phlogiston of 20-th century
(Leonid Bulavin)

Our attention is focused on macroscopic and microscopic manifestations of H-bonds in water, firstly, on the behavior of the specific volume and evaporation heat per molecule, heat capacity of liquid and vaporous water, coefficients of self-diffusion and kinematic shear viscosity, dipole moment and the shift of frequency for longitudinal vibration of $O-H$ bonds ect.

From our analysis, it follows that the intermolecular potential for water can be considered as the sum of contributions:

$$\Phi(r,\Omega)=\Phi_R(r,\Omega)+\Phi_D(r,\Omega)+\Phi_E(r,\Omega)+\Phi_H(r,\Omega)$$

describing the repulsive, dispersive and electrostatic interactions correspondingly, as well as H-bonding. For two contacting molecules ($r \sim \sigma_w$) these contributions are in the relation:

$$|\Phi_D(\sigma_w,\Omega)|:|\Phi_E(\sigma_w,\Omega)|:|\Phi_H(\sigma_w,\Omega)|\approx 1:10:1.5$$

The combination

$$U_H(r,\Omega)=\Phi_E(r,\Omega)+\Phi_H(r,\Omega)$$

is often identified with the potential of H-bond, although it lead not frequently to many ambiguitys. In particular, the correct description of the mobility of water molecules and ions in electrolyte solutions in the framework of such a picture is impossible.

General conclusions: 1) H-bonds in water, alcohols and other systems arise due to weak overlapping of their electron shells; 2) their contributions to intermolecular interactions are relatively small and can be taken into account with the help of perturbation theory and 3) main role in the formation of specific of water structure and other properties belongs to electrostatic interactions.

Properties of nano-scale fluctuations and correlation functions based on "comprehensive scaling" approach

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For an integrated description of the properties of critical fluid a new approach, "comprehensive scaling" [1], has been proposed. The symmetric algebra of fluctuating variables has been developed in the fluctuation region. The resulting equations of state and phase diagrams adequately describe the experimental data of inhomogeneous [2] and homogeneous critical fluid for thermal and calorific quantities, thermodynamic responses and kinetic coefficients for all close vicinity of the critical point. Proposed approach gave the possibility to describe the asymmetric internal electromagnetic field in the critical fluid induced by the gravity field [2, 3, 4].

Interactions of the molecules within the fluctuations of the order parameter are indirect collective interactions [5]. Based on the symmetric algebra of fluctuating variables the correlation functions of different orders have been proposed. The proposed unary correlation function of the local density is a density profile within the nano-scale fluctuation of the order parameter. It has been shown that the average density inside of fluctuation is $\rho_a > 2\rho_c$ (ρ_c is the critical density). This conclusion is in agreement to the conclusion $\rho_a \approx 3\rho_c$ follows from the van der Waals model of real gas of fluctuations of the order parameter [2, 6], with the calculations [4] on the base of the fluctuation theory of phase transitions and with the results of spectroscopic experiments.

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An influence of strong correlated states on the optical properties of $Sn_2P_2S_6$ crystal

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$Sn_2P_2S_6$ (SPS) crystal is known as a ferroelectric-semiconductor, photosensitive in the red and near-infrared spectral ranges with promising photovoltaic [1], electrooptic [2] and piezoelectric [3] characteristics. Its physical properties (e.g. conductivity) strongly depends on the crystal stoichiometry [4]. At the Curie' temperature T_c=337 K the phase transition from ferroelectric (FE) to paraelectric phase (PE) is observed [5].

In presented work, the electronic and optical properties of SPS crystals in FE and PE phases were studied theoretically and experimentally. Using density functional theory (DFT) approach, the energy band structures for both phases were calculated. Influence of Hubbard parameters on calculated electronic properties was predicted and compared for FE and PE phases. Was shown, that Hubbard correction has the influence on strongly correlated states on phase transition. The electronic and optical properties of stoichiometric and non-stoichiometric SPS crystals were also calculated and experimentally investigated. Different vacancies created by deficiency of S, Sn or P atoms of SPS crystals create additional energy bands formed near the Fermi level. In the case of S vacancies, an occupied donor band is created and in the case of Sn and P vacancies, empty acceptor bands were observed. In addition, the non-stoichiometry affects the crystal absorption spectra calculated for different polarization. Results obtained theoretically were compared to the experimental data.

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Squaraine-based Brownian quadrupole photomotors

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Brownian motors which convert chaotic Brownian motion to directed particle transport [1] involve a particle (or a large molecule) switching between two (or more) states, with its potential energy asymmetrically changing in space at least in one of the states. If the states are interswitched by light, the corresponding nanodevices belong to Brownian photomotors [2, 3]. In the previously developed Brownian photomotor model [4], cyclic photoexcitation causes fluctuations of dipole, quadrupole, and higher multipole molecular moments. Their contributions to motor properties can be varied by an appropriate choice of substrate according to symmetry rules [5].

Here we study photomotors based on symmetric squaraines, neutral planar molecules with two C2 symmetry axes [6]. As they have neither a charge nor a dipole moment, their multipole expansion is dominated by a quadrupole moment, and they can be called quadrupole photomotors. According to symmetry rules, the motor properties of quadrupole molecules should be most pronounced on the substrates with asymmetrical electron density distribution. As found, quadrupole photomotors (i) have smaller average velocities of directed motion than dipole photomotors [2] and (ii) provide a high degree of motion rectification in a molecular ensemble.

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Stimulated Raman scattering of Cherenkov-type due to temporal dynamics of self-focusing

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It has been analyzed the effect of self-focusing in Kerr-liquid at the nanosecond range of a laser pulse duration. The results concern the location, velocity and acceleration of a focal point under self-focusing. The effect of a group speed of laser pulses is taken into consideration.

The range the focal point velocity spreads from $-\infty$ to $+\infty$. However, at the output of a long cell filled with Kerr-liquid, the focal point velocity is close to the group speed of light. At the front of the pulse, the focal point velocity is slightly higher than the group speed of the pulse, but is slightly less than the group speed on the rear edge of the pulse. Under the minimal self-focusing distance at the top of a laser pulse, the focal point velocity is zero. An acceleration of the focal point at the exit of a long cell may be almost absent, but at the minimal focal distance, the acceleration has a fixed positive value.

The influence of moving focal point speed and self-phase modulation under self-focusing on frequency-angular radiation spectra of parametric stimulated Raman scattering anti-Stokes component is revealed. The self-phase modulation of both exciting and scattered anti-Stokes radiation is taken into consideration. The creation of broadened anti-Stokes component frequency-angular branches is explained. The most intense frequency-angular branches, which are described by the expression typical to Cherenkov radiation, are generated when the speed of self-focused focal point matches phase velocity of nonlinear polarization on anti-Stokes Raman frequency and phase velocity of scattered axial radiation. In particular, under excitation by nanosecond laser pulses such branches in toluene reach shifts of ≈ -200 cm^{-1} relatively to anti-Stokes Raman frequency.

Peculiriaties of soliton excitations in the In_4Se_3 crystal

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Today a large variety of nonlinear structures has attracted considerable interest due to its application in nonlinear optics. Several phenomena, for instance, ultrashort optical pulses in solid state laser, solitary waves in the discrete atomic systems, optical solitons in fibers, for their explanations demand the inclusion of more higher –order dispersion in the nonlinear Schrodinger equation. It is shown [1] that the higher dispersive effects may cause significant qualitative changes in the dynamics of nonlinear structures. From this point of view, it is of interest to investigate the soliton excitations in the layered In_4Se_3 crystal, for which the nonlinear Schrodinger equation with the fourth-order dispersion takes place [2] owing to the nonstandard dispersion law for charge carriers. As it is known [3], the dispersion law for the In_4Se_3 crystal is characterized by the low-energy nonparabolicity connected with opposite sign of the coefficients at the second and fourth order components of the wave vectors.

In this report, we present new investigations of the space-localized excitations of soliton type in the framework of the nonlinear Schrodinger equation. It is shown that the fourth - order effects are crucial for the formation of solitary waves in the layered In_4Se_3 crystal. The balance between the higher order dispersive terms and nonlinearity, induced by lattice deformation, may leads to the different space localized excitations. They can be stable or unstable depending on the parameters of the dispersion law and the wave vector region. It is found that one- soliton and multisoliton solutions can be realized in the In_4Se_3 crystal.

The parameters of soliton excitations (energy, amplitude, velocity) have been determined. The dynamics of soliton in time was investigated too.

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Generalized dynamics of quasiparticle for the crystals with the unit cell of arbitrary complexity of structure

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The conditions of general description of the dynamic properties of the quasiparticles identical with those for real relativistic particles were analyzed. Such an analysis is an actual today, especially, with the increasing of interest to the properties of graphene and other nanostructures of carbon origin. Development of the traditional applications of quasiparticles also requires a generalized analysis of its dynamic properties. It was shown that such excitations are described in three ways simultaneously. First is quantum. It is gives description of the excitations in terms of wave functions and eigenvalues of energy. The second method is classic in relation to wave momentum. The third method that is derived from the second is also a description of the classical type, but in relation to the other momentum – mechanical. Exactly this description of dynamics of the quasiparticle is similar to the dynamics of the real relativistic particle. Crystals with an elementary cell of arbitrary complexity of structure were considered and it was shown that the dynamic model of Dirac is not exclusive only for graphene. It is being implemented in all crystals as an approximation of the generalized dynamic description of quasiparticles in them. It was set that this model is typical not only for any solids, but for any points of **k**-space (except of points, where dispersive correlations have extremums). In particular, for solids with a simple cubic lattice energy of quasiparticles $E(\mathbf{k})=H(\mathbf{p})$ in neighborhood of some point $\mathbf{p}=\mathbf{p}_0$ is determined by equality:

$$E(\mathbf{p})=mC^2(\boldsymbol{\beta}_0\cdot\mathbf{p})-L(\boldsymbol{\beta}_0),$$

where $L(\boldsymbol{\beta}_0)=mC^2\sum\{(\beta_i^0\mathrm{arcsin}(\beta_i^0)+[1-(\beta_i^0)^2]^{1/2}\}$ ($i=1,2,3$) – wave Lagrangian of quasiparticle, $\boldsymbol{\beta}_0$ its dimensionless speed in a point $\mathbf{p}_0$ (with components $\beta_i^0=\sin(p_i^0)$), $m\equiv\hbar/bC$ – the effective mass of the quasiparticle, $C\equiv b|E_0|/\hbar$ – its maximum speed, b – the lattice constant, E_0 – the energy width of the band of conductivity (excitation band). For solids with a simple cubic lattice generalized correlation of Louis de Broglie was also found: $p^i_m=\mathrm{tg}(p_i)$.

Phonon-polaritons in a diatomic ionic crystal

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The Huang Kun macroscopic theory for continuum description of diatomic ionic crystal is used. A Hamilton operator for system of electromagnetic field and relative shifting oppositely charged lattices is proposed taking into account local field acting on the ions. A statistical operator of the system as a first approximation in the introduced small interaction is found. The dispersion equation for the phonon-polaritons as transverse electromagnetic field waves is obtained. By analyzing the resulting dependence graph, a series of stair-like phonon-polariton modes similar to Bernstein modes is found.

π-electron excited states in semi-empirical local coupled-cluster theory

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Designing new optical materials requires investigations of excited states of long π-conjugated systems. Among systems that are both interesting and potentially applicable as such materials, nanotubes, graphenes, fullerenes, *etc.* should be mentioned. Theoretical investigation of these systems requires an adequate accounting of the correlation effects. Such an accounting can be obtained using the coupled cluster (CC) method. The CC wave function that includes singly and doubly excited configurations (CCSD) allows for describing a significant part of the electron correlation effects. A generalization of the CC method to linear response theory (LR) is one of possible methods for investigating excited states. However, the use of the CC method is limited to rather small systems. Recently we proposed a new π-electron approach for describing large polymeric conjugated systems which is based on the locality of the electron correlation effects. In this approach the conjugated system is represented as a set of unbounded ethylene molecules (cue) and the exact wave-function is described as a superposition of configurations representing inter-fragmental excitations. The use of the cue-CCSD approach allows for a significant reduction of the computational costs. Thus, a possibility arose for theoretical calculations of non-linear optical properties of long polymeric chains [Mol. Phys. **111**, 3779, 2013].

In the present communication we show how our cue-approach can be generalized to perform excited states calculations (cue-LRCCSD). The results of some tests performed with the generalized cue method reveal high accuracy of the approach as compared with the LRCCSD method and the exact full configuration-interaction (FCI) method. Excitation energies for trans-polyenes, C_nH_{n+2}, obtained with the different methods and presented in the table, support this conclusion.

Table. Excitation energy (eV) for trans-polyene B_u^+ state.

n	4	6	8	10	12	14	16	30
LRCCSD	5.75	4.99	4.50	4.18	3.95	3.78	3.65	3.36
cue-LRCCSD	5.75	4.97	4.49	4.17	3.95	3.79	3.68	3.26
FCI	5.76	5.01	4.55	4.24	4.02	3.86	–	–
Exptl.	5.73	4.93	4.41	4.02	–	–	–	–

Models of the Pt-based catalysts for the direct oxidation of the methanol fuel cells

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Fuel cells, especially low temperature fuel cells are clean energy devices that are expected to help address the energy and environmental problems that have become prevalent in our society. Pt-based alloys developed for many years to improve the catalytic activity of the oxygen reduction reaction and the methanol oxidation reaction. Great progress has been made in recent years in terms of alloy activity screening, alloy mechanism discovery, and alloy stability investigation. On appeling aspect of bimetallic catalysts is the possibility of rationally designing of the materially changing the layer elements and composition [1-3].

The main research methods are theoretical calculations based on the density functional theory and the pseudopotential method using the author program code. We use slab geometry to model the layer catalyst, using Pt, Ni, Cu layers for the (100) epitaxial heterostructure with mechanical strain or Pt-Ni, Pt-Cu alloys on surface of which the adsorption structures are created, on two side on the slab. Theoretical calculations illustrates that the mechanical stress and the presence of dissociated oxygen have the greatest impact on increasing electron bimetallic catalyst activity during the oxidation of methanol with using bimetallic layered mechanically strained Pt,Ni,Cu-based catalysts, which have a variable composition. Because of various stable arrays of platinum and nickel formed pressure gradient, accompanied d- and f- overlapping orbitals increasing the catalytic activity, increases the chemical and adsorption activity of the film.

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Determining of structural properties of model fluids by numerical solution of the equations of motion for the Fourier coefficients of density fluctuations

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Structural properties of two-dimensional Gaussian model fluid were investigated by the method of collective variables in the harmonic approximation.

Internal energy, system of many particles and radial distribution function of model fluids in microcanonical ensemble were evaluated with molecular dynamics method.

In order to ensure that the system established thermal equilibrium, the energy value was observed at each time step. For two-dimensional models of fluid particles with Gaussian interaction were constructed. The effect of harmonic approximation to the description of structural properties was noted.

Correlation functions and associated relaxation times in the model of resonant tunnelling driven by cross-correlated colored noises

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One of the fundamental problems in study of the dynamics of nonequilibrium systems is the investigation of their behaviour under the influence of noises of different nature. It is reasonable to suggest that fluctuations of some parameters can lead to noises of additive as well as multiplicative character which are not independent. They can have common origin and therefore correlate with each other. At present time much attention is paid to the investigation of noises with finite correlation times (colored noises) that in some cases allows to achieve a more realistic model for describing the system. As the dynamical characteristics of fluctuations in stochastic unstable systems, correlation functions in a nonequilibrium steady state and the associated relaxation times are often used.

We have studied the effects of cross-correlated noises on the process of relaxation of fluctuations in the model of resonant tunneling in which noise sources due to incident flow intensity fluctuations and frequency fluctuations were assumed to exist. The normalized correlation functions and associated relaxation times were calculated with the help of a projection-operator technique with account of memory effects. The influence of noise intensities, their correlation times, and also the strength of correlation between the noises on these functions has been analyzed.

It was found that the strength of cross-correlation between two noises can facilitate the intensity fluctuation decay. The behaviour of the relaxation time with respect to the noises strength can be characterized as a stochastic resonance phenomenon. It was shown that the enhancement of self-correlation time of the intensity fluctuations accelerates the transition from the unstable state while the growth of self-correlation time of frequency fluctuations results in retardation of the transition thereby stabilizing the system.

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