XXI Galyna Puchkovska
International School-Seminar

SPECTROSCOPY OF
MOLECULES AND CRYSTALS

Book of Abstracts

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The Book contains abstracts of reports presented at XXIth Galyna Puchkovska International School-Seminar “Spectroscopy of Molecules and Crystals” (22-29 September, 2013, Beregove, Crimea, 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.
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В збірнику представлені тези доповідей XXI Міжнародної Школи-семінару імені Галини Пучковської “Спектроскопія молекул і кристалів” (22-29 вересня 2013 р., Берегове, Крим, 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.
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40-YEAR HISTORY

OF GALYNA PUCHKOVSKA INTERNATIONAL SCHOOL-SEMINAR

“SPECTROSCOPY OF MOLECULES AND CRYSTALS”

The International School-Seminar “Spectroscopy of Molecules and Crystals” has a long history. Founded in 1973, this year’s 21st School-Seminar marks its 40th anniversary. The idea of this scientific event was put forward by a working group from the Institute of Physics, Kyiv, Ukraine. Main architects of the School-Seminar were Chairman, Director of the Institute of Physics, Member of the National Academy of Sciences of Ukraine Marat Shpak, and senior researcher of the Department of infrared spectroscopy, later a Head of Photoactivity Department, Professor Galyna Puchkovska. Among the founders of the School-Seminar was also its Honorary Chairman since 1979, world-known physicist and theoretician, Member of the National Academy of Sciences of Ukraine Alexander Davydov.

The School-Seminar becomes regular biennial meeting of prominent scientists from all over the former Soviet Union. The geography of the School-Seminar covers nearly all famous places of Ukraine. Without doubt, the heart and soul of the school, its organizer and inspirer from the very beginning was Professor Galyna Puchkovska.

The scope of the School-Seminar is broad and covers all aspects of spec-

Galyna Puchkvoska and Alexander Davydov (in the center) at VI SSSMC (1983, Chernihiv)

troscopy including theoretical spectroscopy, molecular dynamics and molecular interactions, spectroscopy of molecular crystals, spectroscopy of inorganic crystals and semiconductors, as well as applied spectroscopy.

The first School-Seminar was held in Western Ukraine near Uzhgorod at the sport and recreation camp of Uzhgorod University "Skalka". About 80 participants from Ukraine, Russia, Belarus and other former Soviet countries took part in this event. For many years, it continues to bring together scientists interested in spectroscopic methods of research from all over the world. Every year the School-Seminar widens the number of its participants. With time, a true family of devotees of Galyna Puchkovska School-Seminar was build between spectroscopists, including famous specialists in the field of spectroscopy of solid state and soft matter, non-linear and laser spectroscopy from different countries.

The aim of the School-Seminar, seen by Galyna Puchkovska as a wide-circle meeting of scientists and engineers, is to examine from different points

Participants of XII ISSSMC (1995, Nizhyn)

Participants of XIV ISSSMC (1999, Odessa)

of view the problems and questions of molecular spectroscopy and its applications, to share the experience and to facilitate joint research in different fields of spectroscopy. Apart from its purely scientific goals, the aim of the School-Seminar was always to support young Ukrainian researches, help them to present their ideas to the international spectroscopic community and to initiate common research projects with European scientists and engineers.

Since 2005 Taras Shevchenko National University of Kyiv is a co-organizer of Galyna Puchkovska School-Seminar. Since that time, the School-Seminar has its permanent residence in the University's Centre of recreation and tourism in the village of Beregove in Crimea. On the proposal of the author, the School-Seminar was complemented with a satellite meeting - a summer mini-school of «Minor Academy of Sciences of Ukraine». The best Ukrainian schoolchildren, winners of All-Ukrainian competition on physics may take part in the work of this school.

During 40 years, School-Seminar of Galyna Puchkovska continues to unite spectroscopists from different countries, strengthen scientific cooperation between Ukraine and the entire world, stimulate exchange of thoughts and ideas, and inspire new generations to contribute to the development of science.

V. Pogorelov
Chairman of International
Advisory Committee

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LECTURES

^{1}H, ^{13}C NMR AND RAMAN SPECTROSCOPY OF PROTON/ DEUTERON EXCHANGE IN IMIDAZOLIUM-BASED IONIC LIQUIDS

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Ionic liquids (ILs)/room temperature ionic liquids (RTILs) can be considered as one of the most successful breakthroughs creating smart materials and multifunctional compositions possessing many appealing features important for the applications in high technologies, including various artificial sensors of new generation, electrochemistry, fuel cells and batteries, (bio-) catalysis, *etc* [1]. On the other hand, the physical understanding of processes in ionic liquids on a molecular level how the certain peculiar properties may arise from the long-range interionic interactions coupled with their structural features and dynamics is still one of the main challenges for fundamental research.

The anion effect on the proton/deuteron (H/D) exchange in the imidazolium-based ionic liquids [$C_n$mim][X], were $n = 4$ and 10, X = I, Br, Cl in D_2O solution was studied applying ^{1}H, ^{13}C NMR and Raman spectroscopy.

The time dependencies of integral intensities in NMR and Raman spectra indicate that the H/D exchange in [$C_n$mim][X] runs faster in sequence of anions Cl, Br and I. The role of anions has been discussed. They interact with cations via H-bonds and bind the water molecules in their solvation shells. The overlap and the competition of these processes may cause complex dependency of the H/D exchange reaction rates on the sample composition. The concept of the conformational changes coupled with the H/D exchange in imidazolium-based ionic liquids can be rejected in the light of ^{13}C NMR experiment and DFT calculation. The revealed changes in ^{13}C NMR spectra are caused by the Nuclear Overhauser Effect (NOE) and the secondary (^{13}C) isotope effect not being the signal shifts due to the conformational *trans*-*gauche* transition.

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NEW ORGANIC PROBES FOR TWO-PHOTON INDUCED FLUORESCENCE MICROSCOPY APPLICATION

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The linear photophysical, two-photon absorption and superfluorescence properties of new organic fluorene and squaraine derivatives with great potential for two-photon fluorescence microscopy application have been reported. The steady-state and time-resolved spectral analysis of new molecules were performed in solvents of different polarity at room temperature under CW and pulsed femtosecond excitation. Different types of fast relaxation processes have been detected in the excited electronic states of fluorene derivatives, including solvation dynamics. Efficient superfluorescence radiation was observed for fluorene and squaraine molecules under femtosecond pumping conditions. Two-photon absorption (2PA) spectra of new molecules were obtained in broad spectral range using open aperture Z-scan methodology and the maxima values of 2PA cross sections up to 2500 GM were shown. A potential application of new probes in bioimaging was demonstrated via one- and two-photon fluorescence microscopy techniques.

COMPLIMENTARY INVESTIGATION OF MICROSTRUCTURE OF IONIC SOLUTIONS BY NMR-RELAXATION, QUANTUM CHEMISTRY AND MOLECULAR DYNAMICS METHODS

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Nuclear magnetic resonance is a fruitful tool for the investigation of the internal structure of ionic solutions, and NMR-relaxation plays an important role. Spin-lattice relaxation rates of ^{1}H, ^{2}H, ^{7}Li, ^{13}C, ^{23}Na, ^{35}Cl, ^{81}Br and ^{127}I nuclei in electrolyte solutions and ionic liquids were measured in a wide temperature range using the Bruker SXP 4-100 and AVANCE 500 spectrometers. The NMR-relaxation method for the investigation of aqueous salt solutions was earlier developed in [1]. The change of quarupole coupling constants (QCC), caused by the deuteron transfer from water molecules to D_3O^+ ions, and the change of the QCC of deuterons, which belong to water molecules in hydration shells of “strong” ions, were detected.

In order to conciliate the data obtained from proton and deuteron resonances, the electric field gradients and the QCC of deuterons in different molecular complexes were estimated from quantum-chemical calculations. The DFT method with hybrid functional B3LYP was chosen to take into consideration non-local electronic correlation. Flexible basis sets (6-31++G**, 6-311++G**, aug-cc-pVDZ, aug-cc-pVTZ and aug-cc-pVQZ) with diffuse functions were used, that is important for molecular systems with hydrogen bonds.

For the modelling of aqueous solutions the standard molecular dynamics has been carried out. The original combination of classical molecular dynamics simulation and Car-Parrinello method, based on the DFT, is also used.

The work is partly supported by grants of Saint-Petersburg State University and Russian Foundation for Basic Research (Grant No 13-03-01073a).

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GLASS FORMATION AND NUCLEATION IN SUPERCOOLED LIQUIDS

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Glasses, and the supercooled liquids from which they are usually prepared, provide a challenging array of fundamental questions that have been the subject of study for nearly 100 years [1]. Research in this field has been concentrated in the temperature range around and below the conventional glass transition temperature Tg. Here we present selected aspects of our study of the vitrification, nucleation and crystallization in a family of glass-formers such as: 2-biphenylmethanol, benzophenone, orto-bromobenzophenone and salol, by using spectroscopic and differential scanning calorimetry methods. It has been found that in the supercooled liquids of the aforementioned compounds the nuclei emerge during the cooling procedure. The temperature at which the nuclei appear lies at ~ 1.2Tg. The precursors of the nuclei originate in the local-density-fluctuation sites, which are already present in the quenching period of the supercooled liquid. In all our experiments nuclei appears no matter how quickly we cooled liquid (fast quenching or slow cooling). During subsequent cooling below Tg the fluctuating nuclei become an important element of the glass structure. The most fascinating fact is that the crystal symmetry of these formed at low temperature nuclei is not consistent with that of the initial crystal. After melting of the glass state the size of these nuclei increases and cold crystallization into the metastable phases occurs. Our results suggest that the metastable phase tends to nucleate in preference to the stable phase in the vicinity of the glass transition, thus the metastable phase at the nanometric size comprises a glass structure.

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PHOTOPHYSICS AND SPECTROSCOPY OF NOVEL FLUORESCENT NANOPARTICLES AND NANOCOMPOSITES

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The electronic absorption and fluorescence spectroscopy was enriched tremendously on the introduction of new fluorescencent nanoscale materials and nanocomposites [1]. In basic research and in many application areas traditionally explored intrinsic fluorescence of biological macromolecules and cellular pigments and of externally introduced organic dyes are presently in strong competition with these new nanomaterials. Among them are conjugated polymers, semiconductor nanocrystals (quantum dots), up-converting nanocrystals, magic-size clusters of silver and gold, nanodiamonds and carbon dots, etc. They demonstrate diverse photophysical behavior and allow obtaining diverse information being used in analytical tools (as sensors) or when they form images in biological systems. Based on them, functional nanocomposites displaying a variety of useful features and thus extending dramatically the information content of output data can be constructed. With their aid one can modulate in broad ranges the wavelengths of excitation and emission, the lifetimes and anisotropies. The systems with 'superenhancement' and 'superquenching' can be designed. Such unlimited possibilities are offered by combining different types of luminophores based on electronic conjugation, plasmonic effect or excited-state resonance energy transfer [2]. A comparative analysis of spectroscopic properties of new nanoscale materials and of their hybrid nanocomposites is provided with the prospect of applications in fluorescence sensing and imaging.

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[2]. A.P. Demchenko, Methods Appl. Fluoresc. 1 (2013) 022001 (28pp)

DIRECT MEASUREMENT OF PLASMON LIFETIME WITH OPTICAL KERR GATE

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Applications of plasmon for information exchange, field enhancement, sensorics and many others require reliable data on its basic characteristics. Lifetime is among the most important but difficult to measure. Because of large oscillator strength of plasmon its radiative lifetime is in the range of only few femtosecond and usually it is beyond the possibilities of time-resolved spectroscopy. Thus, typically it is estimated from its spectral width with inevitable inaccuracies caused by nonradiative decay and inhomogeneous broadening in the samples of nanoparticles with certain size distribution.

We have succeeded in the measurement of quadrupole plasmon lifetime by means of optical Kerr gate. Experiments were performed at the Center for collective use Femtosecond Laser Complex of National Academy of Sciences of Ukraine. Second harmonic of Ti:sapphire laser excited quadrupole plasmon resonance in colloid solutions of silver nanoparticles and their secondary emission is analyzed. Tailing of the order of 45 fs is attributed to lifetime of quadrupole plasmon and much longer delay in picoseconds range observed in dense samples is interpreted as diffusion-like light propagation caused by multiple scattering.

SEIRA AND SERS SPECTROSCOPY: ADVANTAGES AND DISADVANTAGES

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The enhancement of optical process by a factor $10^2..10^{12}$ near rough metal surface, carbon nanostructures, semiconductors is known already from the end of last century for both optical transitions in adsorbed molecules (Raman scattering (RS) of light, luminescence, IR absorption) and the processes which do not depend on the presence of molecules on the metal surface (for example, second harmonics generation). The effect lies in an essential increase of the intensity of transition (for example, effective cross-section increases by factor $10^5..10^{12}$ for RS – the effect was named as SERS and $10\text{-}10^3$ for IR absorption- SEIRA effect) or efficiency of the process near metal surface. The explanation of the effect is not simple and includes several mechanisms: i) the increase of the electromagnetic field near rough metal surface or island metal films, ii) the increase of the dipole transition moment of the adsorbed molecules, etc. [1].

Despite of great interest to these effects, experimental application is not so simple and sometimes it is very difficult to reach high enhancement in the spectra. Factor of enhancement in SERS and SEIRA is determined by 1) by structure and morphology of metal surface [2], 2) type of the molecules and its organization on the l surface [2], 3) geometry of the experiment, type of the substrate materials etc.

Advantages and disadvantages of enhanced vibrational spectroscopy, numerous experimental data of SEIRA and SERS, including biomolecules and living cells are presented and discussed here.

Acknowledgment: we thank for financial assistance Project STCU 5525 (2012-2013), Ukrainian-Polish Joint Research Project (2012-2014), PIRSES-2012-318617 FAEMCAR, Ukrainian-Russian Project 60-02-12.

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HYDROGEN BOND NETWORKS IN GUANIDINIUM BASED CRYSTALS. THE X-RAY, SPECTROSCOPIC AND QUANTUM CHEMICAL INVESTIGATIONS

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In design of compound with nonlinear optics properties the special role is reserved for organic molecules with delocalized electron system. The molecules have potentially big NLO responses. On the basis of our experiences as molecule with potentially huge NLO properties the ion of guanidine ($C(NH_2)_3^+$) was chosen. This ion is relatively simple chemical species whose structure is related to those of amides and proteins in which there is considerable interest.

On the other hand the guanidinium ion creates in crystals very interesting networks of hydrogen bonds. Some of these systems have 3D structures, sometimes the 2D chains or dimers connected by hydrogen bonds are noticed.

In this presentation the six structures, typical for guanidinium compounds, are described. The detailed studies of hydrogen bonds network in these crystlas are presented. During these investigations the different experimental methods were used. The X-ray crystallographic results are compared with spectroscopic and theoretical studies.

In most cases the obtained from various experimental and theoretical methods results are convergent, but sometimes the huge differences are observed. The reason for which these discrepancies are noticed will be detailed discussed.

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X-RAY SPECTROSCOPY OF CRYSTALLIZED INSULATOR FILMS AND INTERFACES

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X-ray spectroscopy is one of the effective methods of the analysis of the electronic structure, atomic concentration and chemical phase composition of materials. Near edge spectral dependencies of the x-ray absorption coefficient and spectral distributions of the intensity in the characteristic x-ray emission bands reflect the energy distribution of the density of empty electronic states of the conduction band and occupied electronic states of the valence band, respectively. X - ray absorption and emission processes have a local character (associated with hole localization in the core shell) and dipole selection rules for the transitions between the initial and the final state have been worked out. Thus the possibility to obtain the information about local and partial (allowed for certain angular momentum symmetry) density electronic states of the conduction and the valence band is appeared. Such unique information does not possess a single method.

Advantages offered by synchrotron radiation, such as high brightness, coherency, polarization control and photon-energy tunability give a new push to the development of the X –Ray Spectroscopy and now the X –Ray Spectroscopy includes a whole complex of methods, which well developed for study of crystalline structures. On the progress of these methods for nondestructive analysis of the atomic electronic structure of thin crystallized insulator films and buried interfaces will be reported in the talk.

In particular, it will be shown that in some cases X-ray spectroscopic methods can be more sensitive to determination of the degree of perfection of nano-crystalline structures within the range amorphous phase – crystal as compared with methods of diffraction analysis of the surface.

PHOTON-BOSON CONVERSION IN PHOTONIC CRYSTALS AND DIELECTRIC MEDIA

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Photonic crystals are new physical objects, revealing a number of unique physical properties: negative refraction index, essential lowering of the group velocity of electromagnetic waves, localizing of photons inside the photonic crystals and others. In this work the properties of photon-boson conversion effect in 3D-photonic crystals have been investigated. The dispersion laws of photonic and polaritonic branches of globular photonic crystals and dielectric media have been calculated. Down and up photon-photon conversion phenomenon experimental results for globular photonic crystals are presented. As the sources of exciting light for conversion effect observation the different lasers and spontaneous sources of light have been used: pulsed Nitrogen and Ruby lasers, pulsed and continuous YAG:Nd^{3+} (532.0 and 266.0 nm) lasers, light emitted diodes(366.0, 382.0,410.0 nm), continuum emission of visible range. As a result of light conversion processes in photonic crystals the spectrum of exciting light was converted into the region of photonic crystal stop-band. Thus the technique of light energy transformation into some distinct spectral region has been worked out. Such result may be used for solar cells efficiency increase. The properties of scalar boson [1] (paraphoton) and pseudo scalar boson [2] (axion) as elemental particles of dark matter are described. The theory of two photons conversion into paraphotons or axions in vacuum and in media is presented. There is found, that in photonic crystals and in some dielectric media unitons as quasi particles, corresponding to unit value of refraction index, exist. The prediction has been made, that the essential increase of photon – boson conversion efficiency should take place, when uniton emission for conversion exciting in media is used.

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SPECTROSCOPY OF PHONON AND ELECTRON EXCITATIONS AND THEIR SYMMETRY IN CRYSTALS AND PERIODIC NANOSTRUCTURES

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The lecture is devoted to phonon and exciton elementary excitations in bulk crystals such as graphite, $\alpha - ZnP_2$, CdP_2 and in periodic nanostructures such as graphene, single-walled carbon nanotubes by the methods of optical spectroscopy including micro-Raman spectroscopy.

For the first time the methods of construction of irreducible projective representations of space groups of crystals and periodic nanostructures for analysis of energy spectra of elementary excitations have been used. Method of construction of standard factor-systems and irreducible projective representations for all projective classes of space symmetry groups has been elaborated. The two-valued spinor irreducible representations for description of electronic states for groups $6/mmm\,(D_{6h})$ and $422\,(D_4)$ have been built as an irreducible projective representations of projective class K_1.

The dispersion of electron-phonon resonances near Dirac point in one-layer graphene (as diperiodic nanostructure) and its manifestation in micro-Raman scattering has been studied. A new symmetry classification of electron and phonon states in one-layer graphene, which differs from previous consideration, has been developed. It is found that minimum of i-TO phonon branch at K-point is deeper than it is presented in literature.

The fine structure of 2D-band in micro-Raman scattering spectra of single-walled carbon nanotube (SWCNT) has been observed. It is shown that this fine structure is to be related with incoming resonance on SWCNT's van Hove singularities, which provides the dispersion behaviour of 2D band with the energy of exciting photons and additional resonant conditions including the outgoing resonances and warping effects.

POLARON DESCRIPTION OF THE TRIPLET ENERGY TRANSPORT IN CONJUGATED POLYMERS

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The success of organic functional materials in optoelectronics device applications depends on our understanding of the excited state photophysics. At present, there is a particular need to develop our knowledge about the spin triplet excited state, which is used extensively in organic light-emitting diodes (LEDs) and solar cells. In LEDs, triplet states are the major excitations generated in the course of charge-carriers recombination and employed in some device architectures for light emission. Similarly an increasing number of solar cells relies on the diffusion of triplet states to the dissociating interface. Both applications benefit from clever use of the triplet state migration. While much research has been dedicated to the spin singlet excited-state transfer that proceeds through dipole-dipole coupling, the mechanism of triplet motion has received less attention. Triplet migration occurs as a succession of triplet energy transfer processes. The individual transfer is based on an exchange mechanism (Dexter transfer) that is well understood for an individual donor-acceptor pair. However our insight into the mechanism of triplet transfer in a disordered organic solid is still limited to only a few studies.

In my talk I will present a model of triplet exciton diffusion in random organic systems, which considers the interplay between polaronic distortion of the excited chain elements and the energetic disorder. It is applied to describe experiments on triplet diffusion in Pt-atom containing conjugated polymers. The model is based on a Marcus jump rate in terms of the small-polaron concept with a Gaussian energetic disorder treated in terms of effective-medium approximation. We found that in for the weak electronic coupling associated with triplet motion, that is typical for conventional conjugated polymers, the triplet transfer is nonadiabatic. For a critical ratio of polaron activation energy E_a with respect to the energy disorder parameter σ (σ/E_a =0.3), Marcus-type multiphonon transport prevails above a certain transition temperature. At lower temperatures, transport is disorder controlled consistent with the Miller-Abrahams formalism. Theoretical results are consistent with triplet transport in the Pt-containing conjugated polymers. Implications for charge and triplet motion in random organic materials in general are discussed.

EMISSION MÖSSBAUER SPECTROSCOPY: NOVEL APPLICATIONS FOR PROBING STRUCTURAL ORGANIZATION OF METALLOENZYME ACTIVE CENTERS

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The emission variant of Mössbauer (nuclear γ-resonance) spectroscopy (EMS) is a highly sensitive and informative nuclear chemistry technique. The use of the ^{57}Co radionuclide is common in EMS applications in materials science and radiochemistry, but biology-related applications of ^{57}Co EMS have been quite rare. Nevertheless, in many organisms cobalt is involved in diverse enzymatic activities. In our first relevant studies [1–3], the idea of substituting $^{57}Co^{2+}$ (as an EMS-active probe) for the native cation(s) at the cation-binding sites in a metalloprotein was successfully realised for the first time. It gave 'EMS snapshots' of its coordination microenvironment, featured by its Mössbauer parameters. This was demonstrated using, as a representative example, glutamine synthetase (**GS**), a key enzyme of nitrogen metabolism (isolated from bacterial cells, with Co^{2+} as a cofactor [2]).

Our most recent further EMS studies have shown for the first time that ^{57}Co EMS is sensitive not only (*i*) to distinctions in the coordination of Co^{II} at different cation-binding sites within the enzyme active centres [1, 2], but also (*ii*) to the effects of competitive binding of "EMS-silent" Mn^{2+} (a cofactor other than Co^{2+}), thus revealing the possibility of heterobinuclear catalysis for the bacterial GS, and (*iii*) to fine structural changes induced by covalent modifications of the enzyme molecule (via adenylylation of its subunits related to GS activity regulation).

The results obtained are promising for diverse biology-related structural investigations [3, 4] and, in particular, for investigating the molecular mechanisms of metalloenzyme–substrate interactions using the unique possibilities of EMS.

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ABSORPTION AND ACTION SPECTROSCOPY OF LIVING CELLS IN VISIBLE-TO-NEAR IR REGION: EXPLORING MITOCHONDRIAL MECHANISMS OF PHOTOBIOMODULATION (LOW POWER LASER THERAPY)

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This presentation is devoted to exploring cellular mechanisms of photobiomodulation (older terms: low power laser therapy, laser biostimulation). Photobiomodulation is a method used in clinical practice from beginning of 60ties of last century for wound healing, antiinflammation therapy, to name a few. The cellular mechanisms of this therapeutic modality are still not fully clear.

Absorption and action spectra of monolayers of living cells are recorded and their peak positions were compared. A set of experiments modifying these spectra with chemicals was performed. The structure of absorption and action spectra is rather similar, having four peaks in red-to-near IR spectral region near 620, 680, 760, and 820 nm.

The terminal enzyme of mitochondrial respiratory chain cytochrome c oxidase is considered as the photoacceptor in mammalian cells for visible-to-near IR radiation. The primary physical and/or chemical changes induced by irradiation with monochromatic light in visible-to-near IR region in cytochrome c oxidase molecule are discussed. Two mechanisms occurring in cytochrome c oxidase under irradiation are investigated experimentally. These are an increase of electron flow inside of cytochrome c oxidase and a relieve of NO block in the catalytic center of cytochrome c oxidase. A novel mitochondrial light-activated cellular signaling pathway (retrograde mitochondrial signaling) has been described and investigated experimentally. The critical step here is thought to be an alteration of the cellular redox state: a shift toward oxidation due to irradiation is associated with stimulation of cellular metabolism. Our results evidence that cytochrome c oxidase can work after absorption of light as a signal generator as well as a signal transducer in irradiated cells.

SPECTROSCOPIC STUDY OF THE SPIN-CHAIN NICKELATES R_2BaNiO$_5$

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Compounds R_2BaNiO_5 make a family of isostructural rare earth (RE, *R*) nickelates with S=1 chains (Ni^{2+}). Among them, Y_2BaNiO_5 possesses only one magnetic ion and is recognized to be model Haldane system without magnetic ordering. Magnetic RE ion R^{3+} in R_2BaNiO_5 standing between chains leads to an interchain interaction and results in a 3D magnetic ordering at low temperatures (Neél temperatures T_N ~ 12-60 K depending on *R*). The interest to the R_2BaNiO_5 compounds is kept as 3D magnetic properties coexist with Haldane gap. In this presentation we emphasize the importance of the spectroscopy data for analyzing of magnetic properties of compounds under study.

We present the study of crystal field (CF) in R_2BaNiO_5 by means of temperature-dependent absorption spectroscopy of RE energy levels and CF calculation. The CF effects [1,2] influence the magnetic anisotropy of RE ion and, finally, the magnetic structure of compound. We present also the results of the developed by us a method of Er^{3+} probe for studying of the magnetic structures. The comprehensive study of phonon spectrum of Gd_2BaNiO_5 and first experimental study of phonon-assisted magnetic absorption for Haldane-chains will be presented and the quantum critically behaviour in magnetically diluted mixed nickelates $(Nd_xY_{1-x})_2BaNiO_5$ will be discussed

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PERCOLATION AND DISPERSION OF CARBON NANOTUBES IN DIFFERENT LIQUID CRYSTALLINE HOSTS

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In last decades, the liquid crystalline materials doped with carbon nanotubes (NTs), attract great attention. E.g., the effects of reduction of the response time and driving voltage, suppressing of the parasitic back flow and image sticking, the electro-optical memory effects, ultra-low percolation thresholds were recently discovered [1]. Particularly interesting are LC composites based on nematic, smectic and cholesteric (chiral) liquid crystals (CLC). However, the good functional ability of such composites is determined by dispersing ability and integration of NTs networks into the LC matrix. This work discusses the dispersion, self-organization and percolation behaviours of NTs in different LC host media. The methods for improving of dispersion of NTs are reviewed. The effects of the nano-plates on the dispersability of CNs and positive impact on physical properties of the CN+LC composites are analyzed. Different examples of electro-physical, rheological and percolation behaviour in these systems are considered. The excluded volume theory and methods of computer simulation are applied for prediction of the percolation behaviour in disordered and partially ordered composites [2]. The dependencies of the percolation threshold versus the dispersion state and homogeneity of spatial distribution of NTs are also reviewed.

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DISPERSIONS OF CARBON NANOTUBES IN LIQUID CRYSTALS: FROM MOLECULAR MODELS TO THE DEVELOPMENT OF FUNCTIONAL NANOMATERIALS

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Dispersions of carbon nanotubes (CNT) in nematic liquid crystals (LC) are known as promising materials for a number of practical applications. The main problem is that CNTs, when homogeneously dispersed in LC media (e.g., by ultrasonication), at concentrations above ~0.05% tend to form, in minutes or hours, quasimacroscopic aggregates.

We carried out studies of CNT aggregate formation in LC of different types by a set of independent experimental methods (microscopy, optical transmission, differential scanning calorimetry, conductivity vs time and voltage, methods of singular optics, etc.). Simple methods for monitoring of the aggregation process could be proposed, and a molecular model describing interaction of CNTs with formation of aggregates of fractal nature was developed [1,2]. Such aggregates are designated as "S-aggregates", to distinguish them from, e.g, CNT bundles often observed in not well dispersed samples.

Basing on our understanding of the physical picture of CNT aggregate formation processes, several ways were proposed that would allow suppression of CNT aggregation, thus increasing the time stability of composite nanomaterials based on LC+CNT dispersions. Special attention is paid to "hybrid" dispersions, containing, alongside with CNTs, nanoparticles of different anisometry (e.g., exfoliated plates of montmorillonite-type clays), and to CNT dispersions in cholesteric LC of different nature (induced cholesterics, i.e., nematics with chiral dopants, and "steroid" cholesterics based on cholesterol esters) [3,4].

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PECULIAR POINTS IN THE PHASE DIAGRAM OF WATER-ALCOHOL SOLUTIONS

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The work is devoted to the investigation of nontrivial peculiarities of phase diagram for dilute water-alcohol solutions. Analyzing the temperature and concentration dependencies of the contraction and the adiabatic compressibility for them it is shown the existence of specific points, so called the peculiar points of water-alcohol solutions. The rigorous thermodynamic definition of the peculiar point is given. It is established the integrated principle of corresponding states for the contraction. The statistical theory explaining nontrivial behavior of the contraction and other thermodynamic quantities near the peculiar points is developed. It is shown that the percolation cluster from elementary molecular complexes is formed near the peculiar point. The molecular complexes are the natural elements of structure for water-alcohol solutions and they are formed due to intermolecular interactions, which are stronger for different molecules than for molecules of the same type. It is shown that fluctuations of concentration anomaly increase near the peculiar point. Different manifestations of the concentration fluctuations in the molecular light scattering, the broadening of Mandelshtam-Brilloin peak, the behavior of heat capacity and so on are investigated. The special attention is paid to the scattering of slow neutrons and specificity of Raman spectra near the peculiar points. Some details of our report can be found in the papers:

[1]. V.E.Chechko, V.Ya.Gotsulsky, M.P.Malomuzh // Cond. Matt. Phys. – 2013, in press.

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NONLINEAR LASER SPECTROSCOPY OF NANOSCALE CONFINED MOLECULAR IODINE

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The high resolution laser spectroscopy is the powerful tool of structure atoms and molecules study [1]. The minute spectral lines width and frequency shifts changes can be measured using technique of super narrow optical resonances in optical spectra. We apply the high resolution laser spectroscopy to the investigation of nonlinear absorption spectra of iodine molecules confined in small pores of synthetic opal. The technique of laser frequency-modulation [2] is used in experiments for accurate measurement of spectral positions of iodine hyperfine transitions in visible region.

The synthetic opal matrices were formed both as bulk and film samples and filled by iodine vapour using vacuum sublimation technique. The iodine molecules confined in opal pores have been interacted with pore walls and molecular motion was restricted by sub-wavelength sized pore volume. The effects of molecules confinement in opal pores on spectral structure were studied.

The single frequency diode laser (Toptica Model DL100) at 640-nm has been used for study of iodine nonlinear absorption and dispersion resonances and Renishow Inc. inVia Raman microscope for investigation of Raman spectra of iodine doped synthetic opal. The effects of molecules-molecules and molecules-walls collision on nonlinear absorption resonance frequency shift and linewidth were investigated. The relation of photon crystal-like properties of synthetic opal and iodine Raman spectra features were studied.

The results can be used in the laser metrology and precise laser spectroscopy.

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X-RAY SPECTROSCOPIES AND SCATTERING APPLIED TO WATER: WHAT CAN WE LEARN FROM EXPERIMENT AND SIMULATIONS?

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I will discuss recent experimental and simulation data from x-ray absorption (XAS), emission (XES) and scattering (XRD and SAXS) of liquid water and the picture of fluctuations between high-density (HDL) and low-density (LDL) liquid this has led to [1,2]. Such a two-liquid scenario would explain many anomalous properties, *e.g.*, density maximum, heat capacity and isothermal compressibility minima, but no direct connection has been found to simulations of ambient water. Applying the local structure index (LSI) of Shiratani and Sasai [J. Chem. Phys. **104**, 7671 (1996)] to the *inherent* structure of TIP4P/2005 water we find a strict bimodality in terms of spatially separated HDL- and LDL-like environments in the simulations at all temperatures and pressures with distributions in agreement with the conclusions from XAS and XES, *i.e.* 75% HDL and 25% LDL-like at ambient conditions [3]. The SAXS signal is connected to density fluctuations in the liquid which for water decrease (as measured by the isothermal compressibility) down to 46 ˚C but then increase as the liquid is further cooled. Comparing computed and measured SAXS from ambient down to supercooled (-21 ˚C) temperatures shows excellent agreement at 5 ˚C but increasingly underestimating the SAXS signal upon further cooling, indicating that structural fluctuations at cooler temperatures are underestimated in the simulations [4]. Going into "No man's land" to do experimental measurements has recently become possible through the Linac Coherent Light Source (LCLS) x-ray free-electron laser at SLAC by exploiting evaporative cooling in vacuum of micrometer-sized water droplets from which a full diffraction pattern of individual droplets is obtained through the 100 fs fully coherent x-ray pulses delivered by the LCLS showing a continuous development towards an LDL liquid down to at least 223 K.

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WILSONS $\vec{S}$ VECTORS AND EXACT FORM OF VIBRATIONAL HAMILTONIAN

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In the Born-Oppenheimer approximation the Hamiltonian for molecular vibrational-rotational-translational motion has following form:

$$-\frac{\hbar^2}{2}\sum_{i=1-N}\frac{1}{M_i}\left[\frac{\partial^2}{\partial^2 x_i}+\frac{\partial^2}{\partial^2 y_i}+\frac{\partial^2}{\partial^2 z_i}\right]+U(x_1;y_1;z_1;x_2;....z_N) \qquad (1)$$

where $x_i;y_i;z_i$ Cartesian coordinates of i-th atom. If we have three atomics molecule 1-2-3 and only two stretching coordinates $q=q_{12}$ and $Q=Q_{23}$ are interested us we can get:

$$\frac{\partial^2}{\partial^2 x_1}=\frac{\partial^2 q}{\partial x_1^2}\frac{\partial}{\partial q}+\left(\frac{\partial q}{\partial x_1}\right)^2\frac{\partial^2}{\partial q^2} \qquad (2)$$

Since (2) holds for y_1 and z_1 we can get:

$$-\frac{\hbar^2}{2M_1}\left[\frac{\partial^2}{\partial^2 x_1}+\frac{\partial^2}{\partial^2 y_1}+\frac{\partial^2}{\partial^2 z_1}\right]=-\frac{\hbar^2}{2M_1}\left[\frac{\partial^2 q}{\partial x_1^2}+\frac{\partial^2 q}{\partial y_1^2}+\frac{\partial^2 q}{\partial z_1^2}\right]\frac{\partial}{\partial q}-\frac{\hbar^2}{2M_1}\left[\left(\frac{\partial q}{\partial x_1}\right)^2+\left(\frac{\partial q}{\partial y_1}\right)^2+\left(\frac{\partial q}{\partial z_1}\right)^2\right]\frac{\partial^2}{\partial q^2} \quad (3)$$

Since Wilsons $\vec{s}$ vectors [1] defined as $\vec{s}_1^{\,q}=grad_{r_1}q=\frac{\partial q}{\partial x_1}\vec{i}+\frac{\partial q}{\partial y_1}\vec{j}+\frac{\partial q}{\partial z_1}\vec{k}$

we can rewrite (3):

$$-\frac{\hbar^2}{2M_1}\left[\frac{\partial^2}{\partial^2 x_1}+\frac{\partial^2}{\partial^2 y_1}+\frac{\partial^2}{\partial^2 z_1}\right]=-\frac{\hbar^2}{2M_1}div_{r_1}(\vec{s}_1^{\,q})\frac{\partial}{\partial q}-\frac{\hbar^2}{2M_1}(s_1^q)^2\frac{\partial^2}{\partial q^2} \quad (4)$$

Similar equation we can write for Q and $\vec{r}_3$:

$$-\frac{\hbar^2}{2M_3}\left[\frac{\partial^2}{\partial^2 x_3}+\frac{\partial^2}{\partial^2 y_3}+\frac{\partial^2}{\partial^2 z_3}\right]=-\frac{\hbar^2}{2M_3}div_{r_3}(\vec{s}_3^{\,Q})\frac{\partial}{\partial Q}-\frac{\hbar^2}{2M_3}(s_3^Q)^2\frac{\partial^2}{\partial Q^2} \quad (5)$$

Since second atom involved in determining both q and Q internal coordinates equation similar to (4) and (5) for this atom more complicated. Some special cases of the molecular vibrations were considered and expressions for the exact vibrational Hamiltonian using Wilsons $\vec{s}$ vectors were found.

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HALF A CENTURY OF THE LASER ERA: LASER HISTORY IN THE USSR AS SEEN BY A PARTICIPANT

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The first laser has been put into action by T. Maiman in 1960, using a ruby crystal. This event was preceded by an intensive research in both the USA and the USSR. In particular, the creation of a maser was a very important step, later on awarded by the Nobel Prize in Physics. This Prize was given to N.G. Basov and A.M. Prokhorov from the Lebedev Physical Institute (FIAN) and to C.H. Townes from the Columbia University. Since 1958, several research groups in FIAN actively developed different laser ideas. The first (?) ruby laser in the USSR started to generate in the Laboratory of Luminescence of FIAN in 1961.

At that time, I came to this laboratory as a student of the Moscow Institute of Physics and Technology and began to take an active part in the investigation of the properties of the ruby laser light. I'll share with you my memories of that time and of outstanding scientists I met. I'll also mention that from the very beginning of the laser era, the research in the field of quantum electronics was led also in the Institute of Physics in Kiev.

UNUSUAL PROPERTIES OF WELL-KNOWN MOLECULES

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Rapid development of methods of quantum chemistry and power of computational facilities creates a real opportunity for calculations bigger and bigger molecular systems. This leads to illusion that we know everything about properties of such molecules.

It is well known that benzene molecule has highly symmetrical planar geometry. However it was demonstrated that aromatic ring of benzene is quite flexible [1]. Transition from planar equilibrium geometry to a non-planar one with values of endocyclic torsion angles ±20° results in energy increase by less than 2.5 kcal/mol. More detailed investigation of conformational dynamics of isolated benzene by Car-Parinello molecular dynamics (CPMD) method demonstrated [1] that population of planar geometry of ring is only about 7%. Conformational state of benzene in gas phase may be described as mixture of two symmetric families of boat and twist-boat conformations where planar geometry represents transition state between these two families. Destabilization of planar geometry of ring is caused by significant decrease of entropy of molecule in highly symmetric equilibrium geometry [2].

According to general viewpoint the conjugation between the double bonds in acrolein is stronger than in butadiene because of high polarity of π-system. However, this conclusion does not agree with elongation of central single C-C bond. Detailed analysis of intramolecular interactions in acrolein revealed [3] that length of the single C-C bond in acrolein is affected significantly by n→σ* hyperconjugation between one of lone pairs of the oxygen atom and antibonding orbital of the C-C bond. This leads to elongation of this bond as compared to butadiene despite of stronger π-π interaction between double bonds.

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PHOTOLUMINESCENCE OF C_{60} DOPED WITH MOLECULAR HYDROGEN

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Interstitial voids in the crystal lattice of fullerite C_{60} is large enough to accommodate atoms and smaller molecules. Saturation of C_{60} with various species can drastically change its properties, as it happens with dopants like group I atoms like Li, K, etc. Stuffing C_{60} with chemically neutral species (rare gas atoms and close shell molecules) entails capital changes in the thermodynamics and the lattice dynamics of C_{60}. Hydrogen doped C_{60} still attracts attention of researchers from fundamental viewpoint and as a possible hydrogen storage system.

Photoluminescence spectra of pure C_{60} has been first studied in great detail [1], providing accurate attribution of the rather numerous bands. Using [2] a slightly different method we measured photoluminescence spectrum of C_{60} doped with H_2 to various levels of occupancy over a broad temperature range from 2 to 230 K. In the interpretation of our optical data we utilized the findings of a concurrent structure experiment [3], which enabled us to come to conclusions which put an end to the controversial treatment [4,5] in previous studies of certain effects brought about by saturation. We showed that these effects do not mean that the orientational glass state disappears. Instead, the increase of the orientational glassification point (which we tracked unambiguously) occurs simply because the molecular rotations in a strongly doped sample set in at an appreciably higher temperatures compared to pristine C_{60}. And the main reason behind the drop of luminescence intensity is the break of coherence (caused by rotational jumps of C_{60} molecules) of exciton transport to traps, which makes excitons stop thereby increasing the probability of emissionless quenching.

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THE PHOTOPHYSICAL PROPERTIES OF ORGANIC COMPOUNDS: FROM SINGLE SMALL Pi-ELECTRON CONTAINING MOLECULES TO FUNCTIONAL MACROMOLECULES AND BIOLOGICAL SYSTEMS

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Recently organic pi-electron-containing compounds are in sharp interest of the modern scientific world. This is connected with the search of new materials for nanoelectronic elementary units, the development of materials for information recording and high-effective low-energy light sources (OLEDs), the rising possibilities of biological engineering, etc. The photophysical properties of such compounds are connected with presence of pi-electronic groups in their cells and manifested in the optical (near "biologically active" ultraviolet, visual and near infrared) wavelength range that gives the ground to apply optics spectroscopy for their study.

Our report is devoted to the overview of photophysical and, as the result, functional properties of organic pi-electron-containing compounds. The peculiarities of electronic processes in these compounds are discussed. Main attention is paid to the identification of optical absorption, fluorescence and phosphorescence centers and the dynamics of excitation energy transfer processes in organic compounds. It was proved the system of energy levels of macromolecules could be obtained using the positions of energy levels of monomers. The "exciton" concept is examined, the electronic excitation energy transfer is realized by singlet and triplet excitons. The models of the excitons propagation are discussed, the parameters of these processes (the resulting spreading length and critical length of elementary jump of exciton) are presented.

The applications of photophysics of organic compounds are discussed: molecular (nano-) electronics (the models of functional macromolecules with undirected excitons transfer and our last decisions are proposed), information recording (the parameters of sensitivity and resolution are obtained), chemical engineering (intra-molecular plastification), OLED (the variants of "white" OLED are examined), stabilization of polymers (protection of polymers from photochemical reactions), bridge to biology (photophysical properties, the nature of fluorescence and phosphorescence centers of the DNA, RNA, oligonucleotides, pi-electron-containing proteins and their complexes are discussed).

OPTICAL SPECTROSCOPY OF ISOMERIC TRANSITIONS IN NUCLEUS

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In recent years, much attention is paid to the unique prospect of controlling nuclear matter with optical radiation. The nuclear transition from the isomeric state of the ^{229}Th nucleus to the ground state is of a great interest because the transition wavelength is about 160 nm and this transition is the only known optical transition in nucleus. The very attractive feature of this transition is the possibility to build a very precise nuclear clock. This transition is also very sensitive to hypothetical temporal variation of the fundamental constants.

We present a review of recent activities in this interesting field of optical spectroscopy. We discuss also the possibility of the direct two-photon excitation of the isomeric state in ^{229}Th. We show that the fluorescence intensity due to nuclei excitation is the same for the monochromatic excitation and for polychromatic excitation with a sequence of short light pulses of the same mean intensity. The two-photon excitation of the ion ^{229}Th^{3+} in an electromagnetic trap with a focused laser beam with 320 nm wavelength and 100 mW power can lead to absorption saturation. We expect that an irradiation of crystals doped with ^{229}Th^{4+} with a concentration of approximately 10^{18} cm^{-3} by the field of 10 W laser radiation can result in emission of several photons per second at a wavelength 160 nm. We discuss also the possibility of creation of the inverse population in the ^{229}Th ground-state doublet by means of narrow-band laser.

2

THEORY

MICROSCOPIC DESCRIPTION OF THE WATER'S MOLECULES INTERACTION

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The improved version of the polarizational Stillinger-David potential for intermolecular interaction in water is presented in the work. The new approach for the modeling of the screening function, responsible for the cutting of charge-dipole interaction on small scales, is developed. For the correct description of the long-range asymptote of the intermolecular potential the bare Stillinger-David potential is completed by the interaction between oxygen dipole moments. These improvements of the Stillinger-David potential allow us to reproduce successfully all essential results of quantum mechanical calculations of the interaction energy for water molecules obtained by Clementi.

Analyzing the behavior of the dipole moment for water molecule as a function of inter-particle spacing, we obtain the estimate for two- and three-particle effects in water.

The generalized potential for ion-water molecule interaction in water-electrolyte solutions is proposed. The generalized potential takes into account the additional polarization of the oxygen anion, which appears because of the deformation effects for both ion and oxygen anion at their contact. Due to account of the additional polarization effects the generalized potential for ion-water molecule reproduces the results of quantum-chemical calculations with good accuracy.

The generalized Stillinger-David potential is applied to the investigation of hydration problem.

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CONNECTION OF THE CORRELATION CHARACTERISTICS WITH EQUILIBRIUM AND KINETIC PROPERTIES OF THE CRITICAL FLUID

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Due to the wide use of the unique properties of critical fluid (CF) in the novel technologies, the studies of CF are topical at present time. It requires extensive studies of the equilibrium and kinetic properties of the CF, including equation of state. According to the fluctuation theory of phase transitions [1, 2] the basic equilibrium and kinetic properties of the critical fluid are determined by its fluctuation characteristics: the correlation length R_c, the number N_f of order parameter fluctuations in one mole of a substance, the fluctuation part of the thermodynamic potential of one mole of a substance $F_f=C_0R_c^{-3}$. Due to this, the equation of liquid-liquid coexistence curve, $\Delta c^*=dF_f/d\mu^*=d(C_0R_c^{-3})/d\mu^*$, for the concentration of the binary isobutyric acid - water solution has been studied in the work by the phase diagrams method.

The equation of viscosity, $\eta=\eta_r+\eta_f= A \exp(B/T) + \eta_f(R_c)$, for this solution has been at the same time studied by capillary viscosimeter method. The equation for critical viscosity η was used to describe the temperature dependence of the viscosity. It takes into account the exponential behaviour of the regular viscosity η_r and the fluctuation part of the viscosity η_f, taking into account the spatial dispersion of the system.

It has been shown that the equation of the regular part of the viscosity along the coexistence curve has a form similar to the coexistence curve of the studied solution in terms of concentration. It has been concluded that the similar behaviour of the thermodynamic and kinetic characteristics of the system are connected with their dependences on the correlation length R_c, which is the main characteristic of the substance in the critical region, and determines the behaviour of the physical quantities near the critical point.

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KINETIC MECHANISM OF THE SHIFT OF THE PLASMON RESONANCE OF METAL NANOPARTICLES

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We solve the Boltzmann transport equation for electrons in metal. This allows us to obtain the spatially dispersive permittivity of metal in the forms of the Lindhard longitudinal and transversal dielectric functions (generalized by Kliewer and Fuchs [1]) and the hydrodynamic dielectric functions. Then, the derived permittivity is used in the generalized Mie theory [2]. Our theory predicts that the plasmon resonance of beams of nanometer-sized silver particles shifts by 0.15 eV in excellent agreement with the experimental data [3]. Thus, a new solution to an old problem [4] is given. We find that silver clusters with diameters smaller than 2 nm do not contribute to the extinction spectra of the beams.

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MOMENTUM DIFFUSION OF ATOMS, MOLECULES AND NANOPARTICLES IN AN OPTICAL TRAP FORMED BY SEQUENCES OF COUNTER-PROPAGATING LIGHT PULSES

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The optical trap based in the interaction of atoms with counter-propagating sequences of short light pulses, proposed in [1], is an alternative to the traps based on continuous laser radiation. The main advantage of such a trap is a weak perturbation induced on atoms by optical radiation. Obviously this advantage is important for spectroscopy. After work [1] light pressure force on atoms in the optical trap was investigated in [2–4].

We analyze the motion of atoms in a trap formed by sequences of counter-propagating light pulses. The nanoparticles with "active" atoms that resonantly absorb laser radiation are also considered. The atomic state is described by a wave function constructed making use of the Monte-Carlo approach, whereas the atomic motion is considered in the framework of classical mechanics. The effects of the momentum diffusion associated with the spontaneous radiation emission by excited atoms and the pulsed character of the atom-to-field interaction on the motion of trapped atom or nanoparticle were estimated. The motion of trapped atom was shown to be slowed down for properly chosen parameters of atom-to-field interaction, so that the atom oscillates around the antinodes of non-stationary standing wave formed by counter-propagating light pulses at the point where they "collide". The methods of investigation and main results are applicable to interaction of molecules that have diagonal Franck-Condon factors with counter-propagating pulse trains.

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NANOLASER EMISSION LINE BROADENING AND SHIFTING

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The concept of spaser as the coherent near-field generator and nanolaser based on nanoscale plasmonic resonators has been successfully demonstrated in number of experiments. We have developed the theoretical framework for basic description of nanolaser emission line broadening and shifting. We also theoretically analyzed the phenomena of linewidth enhancement – additional line broadening due to the resonator noise.

The very high material gain needed to compensate for the losses of metal generates extremely strong cavity mode dispersion. This results in giant frequency pulling effect. We saw that frequency pulling effect allows to estimate the material gain of nanolaser simply by measuring the Fabry-Perot mode spacing. In conventional lasers this is quite difficult to do as the effect is extremely small, however, in plasmonic laser this effect is quite pronounced, as shown in our report.

We have developed the density matrix model of the nanolaser and obtain the analytical expressions for the linewidth of the nanolaser radiation, which is valid at any pumping rate. We have shown also that plasmonic nanolaser is truly thresholdless device, due to the extremely strong coupling of the plasmonic mode and the active medium.

The main idea of the theory of linewidth enhancement is to introduce the time dependence in the description of nanolaser action through the dispersion of spectral parameters, describing the localized surface plasmon spectrum. This investigation predicts significant linewidth enhancement with order of magnitude broadening of the output spectrum.

The developed theory could be potential interest to rapidly developing nanoplasmonic devises with incorporated gain /1-3/.

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ONE PHOTON SCATTERING BY AN ATOMIC CHAIN IN ONE- AND TWO-MODE RESONATOR

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In this work a chain of *N* identical two-level non-interacting atoms prepared via a single photon Fock state is investigated. The purpose is to obtain information about the state of electromagnetic field and atomic chain in resonance approximation. The state amplitudes of the atomic system are calculated for several space configurations of the atoms.

Assuming the distances between atoms are quite large, so that the interaction between atoms is negligible, we prepare an ensemble of the two-level atoms initially in the ground state. A single mode of the radiation field is excited in a “Fock” state. This is the case of a purely monochromatic wave with zero line width under the consideration. A laser output in single mode operation can approximate this situation due to its high degree of monochromaticity (small linewidth).

Our work differs from the investigations that were presented, for example, in [1] – [3], where it was discussed the photon scattering by a large space homogeneous system with uniform space atomic concentration coupled to a continuum of quantized electromagnetic field modes. We emphasize our attention to one-dimensional space configurations of atomic chains and take into account a resonator with “limited” number of allowed modes in certain direction.

It was shown that the space configuration of an atomic chain, the total number of atoms, and the distinguished by a resonator directions define the behavior of the state amplitude with time.

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PHASE DIAGRAMS OF CORRELATION AND CALORIFIC CHARACTERISTICS FOR HOMOGENEOUS AND INHOMOGENEOUS MOLECULAR LIQUIDS NEAR THE CRITICAL POINT

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The problem of constructing the phase diagram of thermodynamic characteristics of critical fluid is today an important but also quite controversial. Using the model of the system near the critical point as the van der Waals gas of fluctuations [1,2] of the order parameter in the frame of parametric scaling [3] has been used campaign [4] to the determination of surfaces of thermal parameters for molecular liquids.

New method of comprehensive complete scaling for design and analysis of phase diagrams near the critical point for calorific values has been developed on the basis of a system of parametric equations of state [3]. The behaviour of a wide class of homogeneous and inhomogeneous molecular liquids has been analyzed. The order field and the disorder field have been used as the critical fields.

Three-dimensional phase diagrams have been constructed for various thermodynamic responses. The comparative thermodynamic analysis [4, 5, 6] has been made for them. The properties of various thermodynamic potentials near the critical point have been also studied. Analysis of the properties of large-scale fluctuations of the order and the disorder parameters [7] has been carried out using the proposed new version of the algebra of fluctuating values.

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EFFECTIVE FREQUENCY UP-CONVERSION IN PLASMONIC NANOLASER WITH RARE-EARTH NANOCRYSTALS

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About ten years ago we have proposed to use metallic nanoparticle plasmon resonances for enhancement nonlinear optical processes in rare-earth ion doped nanocrystals. During these years many interesting theoretical and experimental works on this theme were been published. Highly photochemically stable nanoparticles, in which up-conversion luminescence can be excited – so-called up-conversion nanocrystals (UC-NCs) – exhibit widely separated (up to 500 nm) narrow luminescence bands in the visible (VIS) region located far from the excitation near-infrared (NIR) laser radiation, and thus can be more easily identified compared to organic luminophores and semiconductor nanoparticles. Due to a deep penetration of exciting infrared (IR) radiation, the absence of parasitic fluorescence of biomolecules and the absence of phototoxicity and photobleaching upon near IR excitation, UC-NCs can be efficiently used as fluorescent probes in biological studies and fluorescence diagnostics (FD). The doping of such nanoparticles with Gd3+ ions provides the additional possibility of combining fluorescence visualization with magnetic resonance imaging.

This year a single-particle spaser design with well-defined and unidirectional stimulated emission and highly effective laser output have been realized. By using a semishell-capped system design, it was shown that the laser emission can be guided and improved over previous spaser designs based on full-shell spasing nanocavity. The optical extinction properties of the semishell resonator (referred to as SSR) strongly depend on the incidence angle, nevertheless, spaser emission exclusively propagates along a specific direction. The power flow from the SSR is one order of magnitude higher than that from its full-shell resonator counterpart (referred to as FSR). Such system opens up a new avenue for applications of high-intensity nanolasers.

We theoretically discussed last approach allowing the use of rare-earth nanocrystals as gain material for the integration within the nanolaser design. Thus, the proposed design is more compatible with semiconductor photonics and can be applied to fabricate lab-on-a-chip photonic circuits.

FREQUENCY-ANGULAR STRUCTURE OF THE STIMULATED RAMAN SCATTERING PARAMETRIC COMPONENTS UNDER SELF-ACTION

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Stimulated Raman scattering (SRS) is widely used to control the shape of optical pulses and their spectra, the statistics of laser radiation and its spatial distribution, to create devices for conjugating the wave front and to amplify weak signals, etc. On the other hand, the parameters of the scattered radiation, especially spectrum, spatial-temporal structure, and coherence, are also an important source of information about the nature of the scattering process itself and properties of the scattering medium.

However, many features of SRS remain unclear. In particular, in self-focusing liquids, even in the nanosecond duration range of excitation laser pulse, the spectral lines broadening of SRS parametric components significantly exceeds the line width of spontaneous Raman scattering. The proposed list of mechanisms, classification of such broadenings is not conclusive and needs further details and additions. In particular, this paper examines the action of self-phase modulation and relaxation oscillations of nonlinear polarization amplitude under self-focusing conditions.

It's theoretically proved that in self-focusing mode of exciting radiation, self-phase modulation, and the relaxation oscillations of amplitude of the nonlinear polarization the frequency-angular structure of the parametric components of SRS has special features. Maximum of radiation energy shifts relative to Raman frequencies and this shift depends on the scattering angle. The largest Stokes shift (about -10 cm^{-1}) of the maximum energy in the spectrum of the parametric components corresponds to the axial radiation and is determined by the size of the focal area, the time of polarization existence and the mismatch of wave vectors of polarization and parametric component. Obtained estimations of self-phase modulation influence on radiation in case of relaxation oscillations show that this influence is insignificant. The effect is interpreted in terms of short-term phase matching.

NANOLASER WITH NONLINEAR ABSORPTION GAS NANOCAVITIES

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Coherent light and surface plasmon generation on nanoscale has recently attracted significant attention due to numerous potential applications in the fields ranging from biosensing to optical interconnects. The physical dimensions of laser are defined by its cavity which generates optical feedback based on constructive interference of propagating waves. Since the interference requires phase accumulation of at least 2π, the resonator dimensions cannot be much smaller than half wavelength in each direction and, in fact, are limited by the classical diffraction. As well known the smallest lasers approaching this limit are Vertical-Cavity Surface-Emitting Lasers (VCSELs).

Conceptually different approaches are required for creation of sub-diffraction coherent light generating systems. One of the promising solutions is based on incorporation of nanometric structures made of noble metals supporting plasmonic excitations. Such structures can confine light far-beyond the natural limit of diffraction by coupling it into coherent oscillations of free conduction band electrons near metal surfaces. The plasmonic effect can confined optical mode in one or two dimensions, while the facet reflections in third dimension can be used to generate sufficient feedback for lasing.

Ideologically new approach to laser resonators was proposed in /1/. It was suggested to replace the interference phenomena by the near-field feedback and in such way it was introduced the concept of SPASER as a coherent source of plasmonic excitations. In a case of efficient coupling of localized surface plasmons (LSPs) in far-field photons, the SPASER can be considered as a nanolaser. This system was successfully demonstrated, employing a core metal nanoparticle and surrounding active dyes.

Our report main new idea is to investigate the opportunity of obtaining coherent radiation from nanometric laser with nonlinear atomic or molecular absorption. We propose some real system and give needed estimations for lasing at sufficiently narrow and frequency stable lines of rear-earth atom in solid and molecular gas in nanocavities. We used the anomalous enhancement of radiation probabilities of molecules near the nanopores as main way to put the lasing at narrow inverted Lamb-dip.

High intensity of nanolasing gives rise to many another nonlinear phenomena as two-photonic absorption and frequency up-conversion that we also would discussed.

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NON-STATIONARY COHERENT EFFECTS IN FREQUENCY-MODULATED FIELDS PROPAGATED THROUGH MOLECULAR GASES

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The affect of non-stationary coherent effects on transmission spectra of molecular gases is numerically simulated in a three-level system with one of the near-resonance fields being frequency-modulated. The numerical model is based on density matrix equations in RW approximation with atomic relaxation properly taken into account and nonlinear wave equations for propagated laser beams – probe and pump. Slow modulation of probe beam is shown to be equivalent to CW excitation with the frequency changed point by point. As the modulation period approaches the relaxation times, the delayed response of the system is shown to cause the coherent population trapping resonance shift and reshaping, as well as the appearance of transient oscillations of the energy level populations, distorted the spectral characteristics.

OPERATING PRINCIPLES OF SINGLE-MOLECULE AND COLLECTIVE BROWNIAN PHOTOMOTORS

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Unlike most of Brownian motor models in which the state of a point particle is described by a single scalar fluctuating parameter, we consider light-induced dichotomic fluctuations of electron density distributions (EDDs) in an extended molecule moving in the electrostatic periodic potential of a polar substrate [1, 2]. This model implies that the potential energy profiles of two motor states differ substantially and their symmetry is dictated by the interplay between the symmetries of the substrate potential and of molecular electronic states. A necessary condition for the occurrence of directed motion, the asymmetry of the potential energy profiles, is satisfied for (i) symmetric EDDs in molecules on asymmetric substrates and (ii) asymmetric EDDs in molecules on symmetric substrates. In the former case, the average velocity of directed motion is independent of molecular orientations and the ensemble of molecules moves as a whole, whereas in the latter case, oppositely oriented molecules move counterdirectionally thus causing the ensemble to diffuse [3]. Quantum chemical data for specific organic-based photomotors demonstrate that the behavior of molecular ensembles is structurally controllable: they can be transported as a whole or separated into differently oriented molecules depending on the ratio of symmetric and antisymmetric contributions to the substrate electrostatic potential and to the molecular EDDs.

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SPECTRAL PECULIARITIES OF POLYMER- DYE NANOCOMPOSITES BASED ON SOME CARBAZOLE DERIVATIVES

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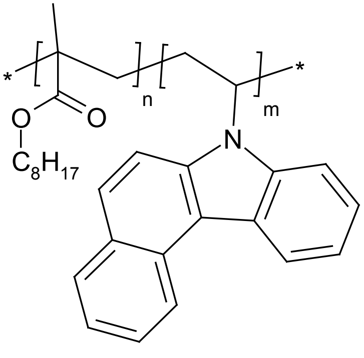
Nowadays ones of the most investigated topics are organic photovoltaics for the green energetics. As a rule polymeric photovoltaics consist of electron-donating polymers that absorb the sun rays, photogenerate charge carriers, and transport the charges and of electron acceptors [1]. The last ones in our work were phthalocyanines and polymethine dyes, as electrondonor polymers we studied PPV and carbazole derivatives. Previously copolymers of n-octyl methacrylate (OMA) with N-vinylcarbazole and N-vinyl-3-iodo-carbazole were studied, now new materials have been found – copolymers of OMA with N-vinyl-7H- benzo[c] carbazole with more conjugated electronic structure:



For these copolymers monomers ratio is 1:1 (m=n) and mol. weight is 7000.

For all copolymers their spectral properties were studied in solutions and in films. The last copolymers have more intensive long-wave absorption than previous ones, the copolymerization causes bathochromic shifts. For films we have found that the nanoparticles are formed as a result of aggregation of dyes molecules in polymer matrixes leading to a bathochromic shift of the absorption of the composite and to an increase in its light sensitivity [2].

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THEORETICAL INVESTIGATION OF SPECTRAL PROPERTIES SOME DYES FOR LUMINESCENT SOLAR CONCENTRATOR

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The European Committee wants all newly built buildings to be near-zero energy by 2020 [1]. This demands architects integrate energy saving and energy generation into their designs. An alternative solar energy harvester was proposed in the 1970's, the luminescent solar concentrator (LSC) [2,3]. The luminescent molecules can be organic fluorescent dyes, or inorganic phosphors or quantum dots.

In this paper we present the results of theoretical investigations by quantum-chemical calculations the spectral properties of some dyes (coumarin 6, Nile red, perylene). These dyes are chosen because of their absorption and emission spectra are situated in different frequency ranges. In addition to the general requirements for all phosphors - a high fluorescence quantum yield, photochemical stability, they must meet the requirements due to the physical aspects of their application, including, low temperature and concentration quenching, resistance to UV radiation. We studied the dependence of the luminescence intensity on the nature of the matrix, which is modeled with solvents of different polarity. It has been observed also that in the presence of the nanoparticles aerosil the intensity fluorescence of dyes molecules is increase as excitation in the UV spectrum and in the visible region. The relationship between electronic structure and nature of polymer matrix has been established.

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THE PECULIARITIES OF CHANGES OF SPECTROSCOPIC PARAMETERS OF EXCITED VIBRATIONAL MOLECULE'S STATES

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The modern resonance methods of a high definition laser spectroscopy define actuality of theoretical investigation of influence perturbations of vibrational states on the peculiarities of changes structurally-dynamic and spectroscopic parameters of polyatomic molecules and also on the predictions of new results and relationships. In this work the analytical method of discrete spectral analysis perturbations theory are developed which is based on modification of the Wilkinson's method of perturbations theory [1], this analytical method is used for a solving of the direct spectroscopic problem of excited molecule's vibrations with given analytical formulation of dynamic coefficients matrix till n degree of components. The obtained results after a solving of the main equation for perturbation vibrations are used for the description of the influence of perturbation vibrations on asymptotic form for changes of frequencies, elements of vibration's forms tensor, structurally-dynamic and vibrational-rotational parameters of polyatomic molecules.

Within a matter of the offered method of a perturbation theory the Arnold's method [2] is used which allows to consider and to estimate the influence of resonance interactions between vibrational modes as kind of Darling-Dennison, Fermi and Douglas-Sharm modes, which connect excited vibrational states with other close situated. The new equations are derived which define the shifts of band's centers, the peculiarities of changing of centrifugal distortion parameters, the Coriolis interaction coefficients, the anharmonic electro-optical parameters, all which are the main parameters in equations for absolute intensities of spectral lines and integral intensities of lines of excited and high excited vibrational states of polyatomic molecules.

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CAPTURE OF MOLECULES WITH DIAGONAL FRANCK–CONDON FACTORS BY SEQUENCES OF COUNTERPROPAGATING LIGHT PULSES

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The optical trap for atoms proposed in [1] is based on the interaction between atoms and sequences of counter-propagating π-pulses. The control of atomic motion with the help of light pulses can considerably reduce the influence of laser field on atoms in comparison with continuous laser radiation. Recently [2] laser cooling of a diatomic molecule (SrF) by continuous laser radiation was demonstrated. The success of the cited work was based on the specific matrix of Franck-Condon factors, which is very close to diagonal. As a result, the interaction of such molecules with laser fields resembles the interaction of two-level atoms. It is well known that two-level atoms can be cooled not only by continuous radiation, but by laser pulses too [3].

We investigate the interaction of close to diagonal Franck-Condon factors molecules with laser fields and show that the sequences of counterpropagating light pulses can form the trap for such molecules if the parameters of interaction with laser radiation (energy and duration of pulses, pulse repetition frequency and detuning from resonance) are properly chosen. Besides that, the molecules can be cooled approximately to Doppler limit. We also discuss another regime of interaction of laser radiation with molecules, when momentum diffusion instead of cooling takes place.

Theoretical background of the study is the Monte-Carlo wave function approach [4]. This approach gives us the opportunity to simulate spontaneous emission. The motion of molecules is described by classical mechanics.

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3-DIMENSIONAL SURFACES OF CORRELATION AND THERMAL CHARACTERISTICS OF HOMOGENEOUS AND INHOMOGENEOUS MOLECULAR LIQUIDS UNDER THE EARTH GRAVITY

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It was established [1,2] by using of model of system near the critical point as Van der Waals gas of fluctuations of order parameter that the dependence of amplitudes of coexistence curve Bn versus critical value of compressibility factor is linear. This work presents results of PVT data analysis of a wide class of liquids which involved analysis of critical indices received by a method of small parameter [3] and determination of amplitudes of the critical isochor, G0, and the critical isotherm, D0.

The equations of a parametrical scaling [4] are used for representation of the equations of state for a critical fluid in a general form in all inner circle. Amplitudes of a, k of the equations of a parametrical scaling are expressed through amplitudes of B0, G0, D0 and connected with the compressibility factor of substance [5].

Using the experimental data the method for design and analysis of phase diagrams at the fluctuation area for homogeneous and inhomogeneous systems under the Earth gravity has been developed on the basis of a system of parametric equations of state [4]. These surfaces were used for finding the three-dimensional surfaces of thermodynamic and correlation parameters of a number of molecular liquids in the fluctuation area.

It was constructed large-scale function of thermodynamic and correlation parameters of uniform and spatially non-uniform molecular liquids at the interval of temperatures $t>0$ and $t<0$.

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COEXISTENCE CURVES OF ION-ELECTRON LIQUIDS WITH CUBIC LATTICE AND ION-ELECTRON MELTS

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The equation of coexistence curve of metals and metal melts in the fluctuation region near the critical temperature has been studied in the work on the basis of the model of gas of order parameter fluctuations with the properties of the real Van der Waals gas [1] by using the values of the critical exponents obtained by the method of small parameters [2].

In the previous studies for the molecular liquids and solutions [3-5] it was shown that the parameters of the equation of state based on the Van der Waals gas of order parameter fluctuations are linear functions of the critical value of the compressibility factor, $Z_c = P_c V_c / RT_c$. The literature data for ion-electron systems [6-11] have been analyzed by the method previously developed and tested for molecular liquids. It has been shown that one-component substances belonging to the group of metals with cubic lattices are characterized by linear dependences of coefficients of the coexistence curve on the critical parameter P_c/T_c. This parameter has a physical meaning of "interaction length" of the particles in the "cell of critical interaction".

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NANOSTRUCTURAL AND CORRELATION CHARACTERISTICS OF CRITICAL FLUID

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The actual mechanism of physical processes, which lead to a wide practical use of the unique properties of critical fluids (CF) in a variety advanced technologies [1, 2], is not yet known till this time. Understanding these processes is essential for choice of technological parameters for their successful practical use and even for the interpretation of global phenomena occurring in the Earth's crust.

The fluctuation theory of phase transitions (FTPhT) [3] is used to explain fluctuation structure of substance in a critical state, the fluctuation mechanism of formation and decay of the order parameter fluctuations. According to FTPhT [3], the main structural features of CF are: the correlation length R_c and the number of the order parameter fluctuations in a volume unit $N_f \sim R_c^{-3}$, the density of substance ρ_f in the fluctuation volume $v_f = 4/3\,\pi R_c^3$. It is these structural characteristics determine the fluctuating part of the thermodynamic potential of the critical fluid $F_f^* = C_0 R_c^{-3}$, its equilibrium and kinetic properties.

In this paper these nanostructural characteristics of CF have been studied using molecular light scattering [4-6]. The obtained experimental data have been used for finding another important characteristic of the CF. It is shown that the density ρ_f reaches values, much larger than the critical density of substance ($\rho_f \geq 3\rho_c$) [7]. Using experimental studies [2] of the formation of nanoparticles Al_2O_3, on the basis of critical fluid H_2O, the velocity of the H_2O molecules $\upsilon \geq 10^7$ cm/s has been estimated in the decay and the formation of the order parameter fluctuations. It was concluded [7] that such large velocities of the molecules are the main reason of manifestation of unique properties of CF on its practical use.

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3

MOLECULES

CHEMICAL IDENTIFICATION OF ATOMS IN ORGANIC MOLECULES BY ATOMIC FORCE MICROSCOPY

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Scanning probe microscopy routinely offers high spatial resolution, in many cases down to the atomic scale [1,2]. It was shown that this technique can be used to chemically identify Pb, Sn, and Si atoms in an alloy [3]. We have applied first-principle calculations to explore the potential of AFM for chemical identification of atoms in organic molecules. As a case study, we focused on phenazine ($C_{22}H_8N_2$). We have calculated the interaction energy between the sample molecule and the foremost atoms of the tip. We have obtained interaction energy curves for different positions of the tip above the molecule. Two types of the tip were used: a copper tip and a copper tip terminated with a single CO molecule.

The interaction energy curves are different for different positions of the tip. This suggests that it is possible to chemically identify C, N and H atoms in organic molecules .

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SOLVENT EMPIRICAL SCALES FOR ELECTRONIC ABSORPTION SPECTRA

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Empirical solvent scales are used to arrange the solvents upon their action on the electronic absorption spectra. Kosower scale is one of known for characterizing the solvent influence on the absorption electronic spectra of dipolar solutes.

Kosower scale reflects in a good manner the solvent influence on the compounds which diminish their dipole moments by excitation, because this scale has been proposed for the complex 1,4 ethyl-pyridine iodide which change the orientation of the dipole moment with 90 degrees. In the ground state of the complex, its dipole moment is oriented perpendicularly on the heterocycle plane, between the heterocycle plane and the iodide molecule. In the excited state the iodide molecule becomes neutral part of the complex and the dipole moment is contained in the heterocycle plane. In these conditions, the interaction energy with the solvent differs from zero only in the ground state of the complex. The effect of the intermolecular interactions is higher in the ground state of the complex. The empirical polarities defined by Kosower can describe the proportionality of the wavenumber in the maximum of the electronic transitions with intramolecular charge transfer causing the dipole moment diminishing. All compounds which diminish their dipole moment by excitation will suffer the similar influence on their electronic spectra.

We compared the solvent action on different classes of cycloimmonium ylids and established correlations between the empirical solvent parameters and structural features of the spectrally active molecules.

HYDROGEN-BONDED CLUSTERS IN ASSOCIATED LIQUIDS

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FTIR spectra of liquid monohydric alcohols from methanol to decanol were registered in the frequency range from 500 cm^{-1} to 4000 cm^{-1}. In the registered spectra of all investigated alcohols the wide diffuse band with the frequency near 3400 cm^{-1} was observed. This band is usually assigned to the vibrations of the bonded hydroxyl groups involved into the H-bond formation.

The processes of the molecular cluster formation of monohydric alcohols were investigated using the matrix isolation technique in argon and nitrogen matrices. The methods of cluster isolation in inert gases matrixes provide the possibility to study individual clusters of different sizes. The gradual transformation of the spectral bands assigned to different vibrations indicates the transformation of the structure of the isolated clusters with matrix heating from 10 to 50 K. The changes in spectra at increasing temperature were analyzed, expecting that such experiments may be considered as the model of structural transformations in alcohols during the gas - liquid phase transition. Main changes with temperature increasing were observed in the spectral regions of stretch O-H and C-O vibrations. At the lowest temperatures the spectral bands corresponding to the vibrations of alcohol monomers were registered, during matrix heating these bands were transformed into the bands assigned to dimers, trimers and larger clusters.

The quantum-chemical calculations of different alcohol clusters were carried out with the program set Gaussian 03 (B3LYP, 6-31G(d,p)). The comparison of the calculated vibrational spectra of the studied alcohols with the experimental IR spectra of alcohol clusters trapped in cold matrices gives the possibility to determine the cluster structure of investigated alcohols.

The work was supported by the State Fund for Fundamental Researches in the frame of Ukrainian-Belarusian scientific project “Spectral manifestations of nanoscale structure formations in associated molecular liquids with hydrogen bonding”.

INFRARED SPECTRA AND CONFORMATIONAL BEHAVIOR OF AMINO ACIDS ISOLATED IN LOW TEMPERATURE INERT GAS MATRIXES

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The study has employed the low temperature matrix-isolation IR spectroscopy and the density functional theory (DFT) and *ab initio* calculations to determine the conformational composition of neutral amino acids. IR spectra were registered for the amino acids isolated in Ne, Ar and Xe matrices. UV irradiation and annealing of the samples were used to distinguish spectral bands of different amino acid conformers. Relative Gibbs free energies of the conformers were calculated at evaporation temperature of each amino acid using the CCSD(T)/CBS level of theory.

We found that at least two conformers of each amino acid are present in the matrices: one with a bifurcated NH_2•••O=C H-bond and one with a N•••H-O H-bond. The presence of several conformers in the matrices results in broadening and/or in multiplex structures of most bands in the amino acid IR spectra. We also investigated influence of the matrix environment on the structure and IR spectra of the amino acids using molecular dynamics simulation and DFT/M05-2X calculations. Common features in the IR spectra of nonionized natural aliphatic amino acids are discussed.

This study clearly demonstrates that accounting for the interconversion between conformers separated by low energy barriers is very important to predict the conformational composition of structurally flexible molecular systems. In the case of amino acids most of the low-energy conformers, which are predicted to have significant populations at the experimental evaporation temperature, actually interconvert in matrices to lower energy configurations and, thus, only a very few conformers are actually observed.

PECULIARITIES OF SOLUTE-SOLVENT HYDROGEN BONDING IN OH-CONTAINING LIQUIDS: FTIR-SPECTROSCOPY STUDY

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Hydrogen bonds play an important role in a variety of chemical and biochemical processes. Special interest from view of hydrogen bonds represents highly self-associated solvents. The most known examples of them are OH-containing liquids (alcohols, diols and water). These solvents present a great practical interest. They have used in different industries due to special physical-chemical properties. OH-containing solvents consist of mixture of associative species of various compositions and structure. Dissolved molecule can form hydrogen bonds with these clusters which lead to a change in solutes reactivity.

In present work we have studied hydrogen bonding of dissolved molecules in aliphatic alcohols, ethylene glycol and water using FTIR-spectroscopy method and headspace gas chromatographic analysis. Different proton acceptors were used as solutes. IR-spectra of ketones, esters and amides in aliphatic alcohols, ethylene glycol and water were measured at different concentrations and temperatures.

Obtained results show, that association degree of all studied solutes are less than 100 % in alcohols and ethylene glycol solutions. The absorption band of the carbonyl group in these solvents consists of at least two components related to free and H-bonded C=O groups. At the same time in accordance with IR-spectra studied solutes are completely H-bonded in aqueous solutions. Obtained from IR-spectroscopy measurements values of complexation degree of proton acceptors in OH-containing solvents are in good agreement with the same data determined from gas chromatographic studies.

Enthalpies of hydrogen bonding of studied solutes in OH-containing solvents were determined using temperature measurements of IR-spectra and solution calorimetry data. Values obtained by two different methods are practically the same. It was shown that enthalpies of hydrogen bonding of ketones and esters with aliphatic alcohols, ethylene glycol and water are positive. The reasons of these unusual results were discussed.

Cooperativity of hydrogen bonding in OH-containing solvents was analyzed.

STUDY OF COMPLEXATION IN CYCLOHEXANE-ETHYL ACETATE MIXTURES BY INFRARED SPECTROSCOPY

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Infrared spectroscopy is powerful tool of investigation of liquid systems. The IR spectra are very sensitive to structural changes caused by intermolecular interactions between the components of solution. Multivariate regression can be used for the determination of quantitative information from IR spectra, such as number and concentration of species in the mixture [1].

Our approach is based on a three-component MCR-ALS analysis of the FTIR spectra of cyclohexane-ethyl acetate solutions. We found that three components are required to obtain a good fit to the data (accuracy better than 1%). The “pure” components were identified as “free cyclohexane” and “free ethyl acetate”, and the third component as “cyclohexane-ethyl acetate complex”. The graphical user interface (GUI) in the MATLAB environment developed by Tauler et al. [2] was used for determination of concentration and spectral matrixes. We used MCR-BANDS GUI [3] to decrease rotational ambiguity of obtained solutions.

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COUPLED PHENOMENON OF RANDOM LASING AND STIMULATED RAMAN SCATTERING IN RHODAMINES AND ITS PECULIARITIES

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Multiple elastic scattering of light in active media promotes initiation of two stimulated processes in dye molecules: random lasing (RL) and stimulate Raman scattering (SRS) which occur simultaneously and influence each other [1]. Up to date there are not understanding what are the basic conditions of this phenomenon occurrence and many its behavior are not investigated.

In previous our investigations we found that SRS and RL occurrence is influenced by pump intensity, scattering efficiency and dye molecule concentration. In presented work we extended our investigation and studied the influence of these parameters more detail. Investigations were held with dyes of rhodamine family: rhodamine 6G (R6G), rhodamine 575 (Rh575) and rhodamine B (RhB) in vesicular polymeric films.

By numerous experiments we shown that SRS in multiple scattering media (MSM) never arises without RL, but the last can arises without SRS. So both effects are coupled and therefore they may be considered as single integrated phenomenon conventionally named SRS-RL. RL plays leading role in SRS-RL phenomenon and much effects on SRS occurrence.

The SRS revealing of investigated dyes is quite different. The first two dyes exhibit well-defined SRS lines shifted by pump wavelength variation. Its intensity is proportional to pump and RL intensity and so they are stimulated by both radiations that indicate of SRS and RL coupling. RhB doesn't reveal SRS lines under any conditions. The reason of this discrepancy is different matching of RL spectra and region of possible Stokes lines evaluated from IR absorption spectra. This region is determined by frequencies of dye molecule bonds and located in yellow (550-585 nm) and red (630-650 nm) regions under 532 nm pumping. Then basic condition of SRS-RL occurrence is RL onset and their spectra coincidence with this region. Other parameters (dye concentration, scattering efficiency etc.) influence on SRS-RL via these options.

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SPECTRAL CHARACTERISTICS OF P-CUMYL-PYRIDAZINIUM-BENZOYL-2,4,6-PICRIL METHYLID (CPBPM) SOLUTIONS

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Binary and ternary solutions of p-cumyl pyridazinium benzoyl-2, 4, 6-picril methylid (CPBPM) were used in order to characterize the visible absorption bands and to attribute them to an intramolecular charge transfer (ICT).

The wavenumbers in the maximum of the visible intramolecular charge transfer (ICT) band of p-cumyl-pyridazinium-benzoyl-2, 4, 6 picril methylid (CPBPM) were used to characterize the first solvation shell of the spectrally active compound in ternary solutions achieved with hydroxyl solvents water, ethanol and methanol. The average statistic weights, p_1 , the excess function, $\delta_{(1)}$, and the preferential solvation constant, k_{12} , were estimated on the basis of the solvatochromic effects of binary hydroxyl solvents water + ethanol and water + methanol in ternary diluted solutions of PPBPM. This study contributes to attribute the intermolecular interactions to universal and specific interactions and to estimate their supply to the total spectral shift.

REACTION OPTIMIZATION IN FACTORIAL EXPERIMENT IN SYNTHESIS OF NEW ANTITUMORAL COMPOUNDS BASED ON 5-NITROINDAZOLE

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In order to obtain new compounds with potential antitumor action, new di-(2-chloroethyl)-amino derivatives with 5-nitroindazole as support, have been synthesized. The compounds have been obtained by reaction of the sodium salts of the 5-nitroindazole with tris β-chloroethyl amine. New organic compounds with alkylating group grafted on indazolic substrate through an ethylene bridge have been obtained.

The reaction optimization was realized in a factorial experiment as a polynomial function and the the reaction yield was studied in dependence of the two relevant variables (temperature and reaction time).

The new compounds has been characterized by elemental and spectral (^{1}H-NMR, FT-IR) analyses.

A series of physical properties (color, crystalinity, solubility, melting point, …) were established the new compounds. A complete characterization has been made applying the quantum mechanical methods from HyperChem package.

This synthesized compounds present antitumor potential in experimental tumors Guerin applied to mice with induced carcinoms. A study of the toxicity has been done and the DL_{50} was established.

OPTIMIZATION SYNTHESIS OF SOME NEW HYDRAZONES FROM 5-NITROINDAZOLES AND THEIR TOXICITY STUDIES

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In order to obtain new substances with a potential tuberculostatic activity, we synthesized some new hydrazones derived from the 5-nitroindazole, through the condensation of 5-nitroindazolyl-acethydrazide with various aromatic aldehydes. Their chemical structure has been verified by the elemental and spectral analysis (FT-IR and ^{1}H-NMR) information.

The reaction optimization has been considered important both for the obtaining with superior yield and for limiting the trials for synthesis of the new compounds.

For this purpose factorial experiments of the 3^2 type was organized for each reaction.

The molecular and structural parameters were obtained with HyperChem package.

This experiment permits to obtain the reaction yield as a function of the second degree in the significant independent variables and to have a three-dimensional, spatial representation of the obtained function.

A study of their toxicity has been done, establishing the DL50 values.

THE VALENT ANGLE ASSESSMENT OF THREE ATOMS MATTER MOLECULES IN GASEOUS AND LIQUID STATES WITH C_{2V} SYMMETRY

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Our research is devoted to the vibrational spectroscopy inverse problem solution that gives a possibility to make conclusions about the investigated molecule geometry. In order to assess the searching valent angle the algorithm was elaborated, based on the gradient descend and the inverse spectral problem of vibrational spectroscopy solving. The valent angle finding based on the usage of inverse spectral vibrational spectroscopy problem is a well-known task, but typical methods of these problem solutions are not applied to molecules of matter in liquid state.

3N-matrix method was chosen all possible methods amount to solve the inverse vibrational spectroscopy problem. The usage of method permits to make no assumptions about the molecule force field, besides this method can be applied to molecules of the matter in liquid state. An vibrations anharmonicity always exists so there is a reason to do a correction caused by the anharmonicity. Anharmonicity constants assessment is an important part of the realized algorithm. Taking molecules interaction into account made it possible to insert noncharacteristic vibration frequencies into calculations. The 3N-martix method usage simplifies calculating of u_3 constant corresponding ω_3 normal vibration. Finding u_1 and u_2 constants is more difficult and realizes by method of steepest descent. In order to find the single-valued inverse spectral problem of vibrational spectroscopy solution a shape parameter must be found. The shape parameter ψ is the angle characterizing vibration ω_1 and ω_2 mixing.

The minimum of such a function y called a divergence parameter was found:

$$y = \sum_{i=1}^{k} \left(1 - \frac{\omega_i^{th}}{\omega_i^{\exp}}\right)^2$$

ω_i^{th} is a calculated theoretically frequency, ω_i^{exp} is a measured experimentally frequency. The defined divergence parameter is a many variable function: valent angle β, anharmonicity constants u_1, u_2, u_3, shape parameter ψ. The valent angle assessment was reduced to the divergence parameter minimization. The β value concerning divergence parameter minimum was interpreted as a desired valent angle. For example $\beta=88{,}8°$ for water molecule in liquid state.

ALCOHOL CLUSTERS IN ARGON AND NITROGEN MATRICES

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The methods of cluster isolation in inert gases matrixes [1] provide the possibility to study individual clusters of different sizes allowing for the tracing of the clustering processes of monohydric alcohols from individual molecules to the hydrogen-bonded network which is typical for liquid alcohols [2].

FTIR spectra of monohydric alcohols (methanol, propanol, hexanol) isolated in argon and nitrogen matrices were registered at different temperatures. The gradual transformation of the spectral bands assigned to different vibrations indicates the transformation of the structure of the isolated clusters with matrix heating from 10 to 50 K. The changes in spectra at increasing temperature were analyzed, expecting that such experiments may be considered as the model of structural transformations in alcohols during the gas - liquid phase transition [3].

Main changes with temperature increasing were observed in the spectral regions of stretch O-H and C-O vibrations. At the lowest temperatures the spectral bands corresponding to the vibrations of alcohol monomers were registered, during matrix heating these bands were transformed into the bands assigned to dimers, trimers and larger clusters.

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VIBRATION SPECTRA EVALUATION OF DYES FROM ITS STIMULATED RAMAN SCATTERING IN MULTIPLE SCATTERING MEDIA

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In a multiple scattering medium (MSM) random lasing (RL) and stimulate Raman scattering (SRS) of dyes interact between them and form integrated nonlinear process RL-SRS. Its common spectrum contains solid and linear components caused by RL and SRS respectively. As SRS in MSM occurs at all Stokes frequencies coinciding with RL spectrum [1] there is possibility to evaluate the corresponding section of the molecule vibration spectrum (VS). It needs decomposition of the spectrum by the solid and linear components. The decomposition must be very accurate because errors of solid component determination much influence intensity and contour of the Raman line. The problem is complicated by RL spectrum sensitivity to pump intensity and dependence of SRS lines intensity on RL one.

According to the properties of SRS in MSM [1] we developed algorithm of dye molecules VS from its RL-SRS spectra. VS was evaluated from experimental RL-SRS spectra $I_{RL}(\omega)$ and its solid component $I_{sol}(\omega)$ as proper nonlinear susceptibility $\chi^{(3)}(\omega) \sim \ln(I_{RL}(\omega)/(I_{sol}(\omega)))$. Central idea is requirement of VS independence on RL-SRS spectra under batch processing of them.

The algorithm includes next steps. Firstly the spectral sections containing Raman lines are removed from the RL-SRS spectrum and the rest of him is approximated by two Gaussians to describe its asymmetry. On the second step $\chi^{(3)}(\omega)$ is computed from each $I_{RL}(\omega)$ and averaged VS was determined. With this spectrum (third step) solid components $I^{1}_{sol}(\omega)$ of each experimental RL-SRS spectra are computed. On the last step one of RL-SRS spectra was randomly selected, approximated by Gaussians with descent method and replace previous one. This step sequence repeated in cycles estimating each time mean discrepancy between next and previous solid components. Developed algorithm achieves the independency of output VS on RL-SRS spectrum over ten steps. Evidence of adequacy this algorithm is good agreement computed and theoretical dependencies of SRS lines intensity on pump.

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SPECIFICITY OF STIMULATED RAMAN SCATTERING IN A DYED RANDOM MEDIA

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Stimulated Raman scattering (SRS) in a dyed random media is revealed only together with random lasing (RL). This feature causes important peculiarities of SRS phenomenon in this media. Investigation of these peculiarities is very important both for understanding of this phenomenon mechanism and its spectroscopic application.

We studied in detail evolution of secondary radiation of rhodamines 6G (R6G) and 575 (Rh575) in vesicular polymeric films subject to pump intensity above RL threshold. Their radiation spectra contain many well-defined SRS lines under pumping of YAG-Nd^{3+} laser second harmonic. All the lines arise only in the range of RL spectrum and correspond to first Stokes component of different molecule vibrations, which is proved by good correlation with their SERRS and IR absorption spectra. Under pump increase they arise in consecutive order from shortwave lines to long wave ones. It occurs simultaneously with longwave broadening of RL spectra caused by reabsorption and reemission of RL radiation. At first the intensity of lines grows rapidly but then it strength to become invariable.

These regularities is explained by the conception of SRS as the CARS-like process stimulated by two-component pump formed by RL radiation at Stokes frequency and incident laser pump. This pump forms driving forces to be resonant with molecule bond frequencies. Due to continuous RL component of this pump the resonant forces arise at all bond frequencies which corresponded to Stokes lines in the range of RL spectrum. Dependency of SRS lines intensity on pump is produced by this broadening also because of the same dependence of RL intensity at corresponded Stokes frequency.

This situation principally differs from plain SRS where observed lines correspond to different Stokes order of single molecule vibration. And successive arising of it is conditioned by energy redistribution from lower order Stokes component to higher one.

FERMI RESONANCES IN C_2F_6

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Up to now data of vibrational resonances in hexafluoroethane (C_2F_6) molecule were unavailable. In the present work IR absorption spectrum of C_2F_6 dissolved in liquid Xe (T=163 K) and liquid N_2 (78 K) are studied. Fermi resonance doublets and multiplets are observed in spectral regions of the modes combined with ν_1 and ν_7 fundamentals.

Both ν_1 (A_{1g}) and ν_7 (E_g) bands are active only in Raman scattering, so in the present work we observe Fermi doublets $\nu_1 \sim (2\nu_6)$ (A_{1g}) and $\nu_7 \sim (\nu_6 + \nu_{11})$ (E_g) in liquid C_2F_6.

The parameters of Fermi resonances, obtained from the experimental data are presented in the Table, where χ is the perturbed frequency splitting, Δ is the unperturbed splitting, R is the relative intensity, W is the interaction matrix element and α_{ijk} is the cubical constant of potential energy.

resonance	ν, cm^{-1}	χ, cm^{-1}	R	Δ, cm^{-1}	W, cm^{-1}	α_{ijk}, cm^{-1}
$\nu_1 \sim 2\nu_6$	1416.3 (1) 1425.0 (1)	8.7 (2)	0.4 (1)	4.2 (5)	3.8(1)	7.6 (5)
$\nu_7 \sim \nu_6 + \nu_{11}$	1221.9 (1) 1239.7 (1)	17.8 (2)	0.6 (1)	9 (1)	8.2(4)	23.2 (9)

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MODELING OF 2,3-DI-O-NYTRO-METHYL-B-D-GLUCOPYRANOSIDE TAKING INTO ACCOUNT THE H-BONDING USING DFT METHOD AND INTERPRETATION OF ITS IR SPECTRUM

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Structural–dynamic model of the isolated molecule 2,3-di-O-nytro-methyl-β-D-glucopyranoside was constructed by DFT method in basis 6-31 G(d) in paper [1]. Using the results of modeling the preliminary interpretation of the IR spectra was held.

At presence work the structure and the IR spectrum of 2,3-di-O-nytro-methyl-β-D-glucopyranoside were calculated taking into account the H-bonding. The structures of dymers of 2,3-di-O-nytro-methyl-β-D-glucopyranoside and structures and spectra of H-complexes of 2,3-di-O-nytro-methyl-β-D-glucopyranoside and ethanol were calculated.

There types of dymers can be realized in the sample. There are cyclic dymer with H-bonds between CH_2-OH group and hydroxyl group (dymer I), dymer with H-bond between CH_2-OH groups (dymer II) and dymer with H-bond between CH_2-OH group and hydroxyl group (dymer III).

The structures and spectra of H-complexes of 2,3-di-O-nytro-methyl-β-D-glucopyranoside and ethanol were calculated. There are H-complex with H-bond between CH_2-OH groups (dymer IIa) and H-complex with H-bond between CH_2-OH group and hydroxyl group (dymer IIIa).

Using the results of modeling the H-complexes we defined the interpretation the measured IR spectrum of the 2,3-di-O-nytro-methyl-β-D-glucopyranoside sample.

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PECULIARITIES OF ELECTRONIC PROCESSES IN THE BORON-CONTAINING EMITTING COMPOSITE LAYERS FOR OLEDs

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One of most effective ways to get the light emitting layers with easy tuning wavelength of emitting radiation is the using of small amount of high fluorescence dopants in suitable matrix. Doping with various dyes can offer a color tuning by exploiting excited-state energy transfer. Thus, design of the new effective dye dopants has gained much attention.

The results of investigations of electronic processes in the novel luminescent dyes are presented. The photophysical properties of these substances were investigated in solutions and as dopants in different matrices. The full interpretation of the absorption and fluorescence spectra has been done using the results of quantum-chemical calculations.

The equilibrium molecular geometry and electron structure of the dye molecules were calculated using the package Gaussians-09. The molecular geometry was optimized by DFT/6-31G(d,p)/B3LYP method, while the characteristics of the electron transitions, HOMO and LUMO MOs were calculated using the TD DFT approach.

The dyes absorption and fluorescence spectra were compared in solution and composite thin films. In comparison with spectra in solutions the fluorescence spectra of the composite films demonstrate similar shape and small shift towards the longer wavelengths. This means that the dyes are not destroyed during vacuum deposition.

Calculated high dipole moment of first electron transition, rigid molecules structure, the high quantum yields and possibility of vacuum deposition are the reasons to believe that these dyes are the perspective materials for using as light emitting layers in OLEDs.

MANIFESTATION OF INTERMOLECULAR INTERACTION AND AB INITIO CALCULATION OF CHARACTERISTICS OF MOLECULAR AGGREGATION IN LIQUID ETHYLENE GLYCOL

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In this work we present results of study of intermolecular interaction in ethylene glycol from spectra of Raman scattering. To make a justified assumption on possibility of formation of aggregated intermolecular complexes and monomeric molecules of ethylene glycol in the liquid and manifestation of this formation in Raman spectra we carried out ab initio calculations of normal vibration frequencies, depolarization ratios of bands, energy of formation, and other physical-optical characteristics for various aggregated complexes of molecules. The calculations were performed in frames of HF-approximation with 6-31G(d, p) basis and total optimization of the geometry of molecules.

It was shown the possibility of H-bond formation between ethylene glycol molecules with formation of dimeric aggregates. In the bond's formation participates hydrogen atom of O-H group of one molecule and one of oxygen atoms of other molecule. According to calculations, the energy of dimer formation is 4,6 kcal/mole.

Analysis of Raman spectra and results of calculation shows that the molecules of ethylene glycol are aggregated by H-bonding, and, moreover, dimers with anti-parallel orientation of molecules are formed. It is interesting to investigate a character of molecular interaction and its manifestation in Raman spectra. The formation of intermolecular bond in liquid ethylene glycol manifest itself in the form of asymmetry of 866 sm^{-1}, 1054 sm^{-1} и 1078 sm^{-1} bands in Raman spectra. The half-width of a complicated band of 1054 sm^{-1} and 1078 sm^{-1} is 57 sm^{-1} and consists of two lines. These bands refer to the plane deformational O-H vibrations. According to calculations, the asymmetry appeared in Raman spectrum is related to appearance of vibrations of aggregates in the high-frequency side of the band of monomers. Since ethylene glycol belongs to the group of polyatomic alcohols, high magnitudes of boiling temperature are explained by intermolecular H-bonding. The influence of H-bonding on physical properties of alcohols is rather significant. Calculations show that ethylene glycol molecules possess dipole moment (~2,73 D for monomer, 6,35 D for dimeric aggregate). The length of H-bond is 2,3 Å. We observe a redistribution of electrostatic charge in dimeric aggregate of ethylene glycol, especially on hydroxyl hydrogen atom that can be explained by electron-donor effect of alkyl group.

THE HYDROGEN BOND IN COMPLEXES OF ANILINE AND ITS DERIVATIVES WITH ORGANIC MOLECULES. COOPERATIVITY AND ANTI-COOPERATIVITY

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Amines and its derivatives play an important role in the biological, physical and chemical processes as included in the composition of dyes, pesticides, and medicines, the properties of which by means of intermolecular hydrogen bonding are realized. Important stage in the study of hydrogen bonds is to evaluate and interpretation of the cooperativity and anti-cooperativity effects.

In present work we used the IR spectroscopy and Quantum-chemical calculations for the study of hydrogen bonds of aniline, N-methylaniline with proton donors and acceptors. Choice of molecules is due to that they are compounds that simulate structural fragments of supramolecular systems.

On the first stage absorbance of free molecules of aniline and N-methylaniline in proton acceptors and proton donor solvents were analyzed. It was shown that obtained N-H frequencies of these substances in proton acceptor, proton donor and inert solvents linearly depend between them.

On the second stage absorption frequency of the N-H groups of complexes of aniline and N-methylaniline with proton acceptors in aprotic solvents were analyzed. It was shown that frequency of the N-H groups of complexes amine with proton acceptors in aprotic solvents are linearly on solvent parameter S_{VW}, responsible for Van der Waals interactions. Deviations in proton donor solvents from linear dependence parameter S_{VW}, due to the cooperative effect in these systems. For the of ternary complexes were estimated coefficients of cooperativity of hydrogen bonds and their analysis in terms of the structure of molecules were carried out.

It is shown that the absorption frequency of the N-H groups of aniline in proton acceptors to deviate from the linear correlations of the parameter S_{VW}, which is related due to anti-cooperativity effects. This result using the approach of quantum-chemical calculations was analyzed. The data obtained of anti-cooperativity effects of hydrogen bonds from structure of the interacting molecules were discussions.

VIBRATIONAL SPECTROSCOPIC STUDY OF γ-BUTYROLACTONE

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Electrolyte solutions based on dipolar aprotic solvents (DAS), in the mixtures with lithium salts or ionic liquids (ILs) are now widely used to develop advanced electrochemical energy storage devices – lithium-ion batteries and supercapacitors.

In this regard, the actual task is the problem of prediction of practically important macroscopic properties of the systems on the basis of the key underlying intermolecular interactions.

In the present paper, within the framework of systematic studies of binary systems based on DAS and imidazolium ionic liquids, we present the results of experimental investigations of Raman spectra of γ-butyrolactone (γ-BL) with 1-butyl-3-methylimidazolium hexafluorophosphate ($[BmIm^+][PF_6^-]$) in the range of 50-4000 cm^{-1}.

The goal of the present study is to explore main interparticle interactions in the selected system by following the evolution of spectral profile of the representative bands. Spectral analysis and assignment was complemented with quantum chemical calculations of relevant molecular structures both in vacuum and within different implicit solvation models.

The main focus of the study has been made on the carbonyl stretching band of γ-BL (around 1770 $cm^{-}1$) since it may reveal details of both solvent-solvent and solvent-IL interactions. Our results show that corresponding spectral profiles are of composite nature containing at least three distinct contributions. The later can be ascribed to monomeric γ-BL molecules and dipolar associates (presumably dimmers). Some indication of contribution of the molecules interacting with IL has been found at low γ-BL content.

We have also analyzed CH stretching region (2800-3200 cm^{-1}), particularly aromatic CH stretching profiles due to imidazolium-ring of cation of the IL. The obtained spectral variations along with results of quantum-chemical calculations are interpreted in terms of competition for cations between anions and solvent molecules in order to establish H-bonding interactions.

The obtained results allow one to design and tune similar systems with desired set of properties.

SPECTRAL INHOMOGENEITY OF LOW-FREQUENCY RAMAN SPECTRA OF WATER AND WEAK AQUEOUS SOLUTIONS OF HYDROGEN PEROXIDE

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Previously it was shown that dynamic susceptibility (DS) obtained from the Raman spectra in the low frequency range from 4 to 320 cm^{-1} of water and weak aqueous solutions of hydrogen peroxide, well described by the approximating function with 9 variable parameters [1-2]. Two Lorentzians describe intermolecular vibrations. From the concentration dependence of these parameters was estimated the size of the modified hydrogen bond network of water molecules in the vicinity of peroxide molecule. The frequency and the width of each Lorentzian are strongly correlated [3]. This was explained on the basis of the model of free oscillations of the classical damped oscillator and of spectral inhomogeneity of these lines [4]. On the basis of this model have been defined homogeneous widths of vibrations associated with their decay time and the resonant frequencies, which are coincided with frequencies of infrared absorption [5].

The obtained value of eigenfrequency of HF oscillation in hydrogen peroxide's solution is 183.6 cm^{-1} with a dispersion of 0.5 cm^{-1} (table value 183.4 cm^{-1}), a homogenious width of the contour is 105.0 cm^{-1} with a dispersion of 4.6 cm^{-1}. The eigenfrequency of the bending mode is 51.3 cm^{-1} with a dispersion of 1.3 cm^{-1} (the table is 50 cm^{-1}), a homogenious width is 36.0 cm^{-1} with a dispersion of 2.4 cm^{-1}.

For water, eigenfrequency the HF oscillation is 184.6 cm^{-1} with a confidence interval (CI) 0.4 cm^{-1}), a homogenious width of it is 102.1 cm^{-1} with CI 1.9 cm^{-1}. The eigenfrequency of the LF mode - 49.9 cm^{-1} with CI 0.4 cm^{-1}, a homogenious width of is 22.0 cm^{-1} with CI 0.8 cm-1. Attention is drawn to the significant increase in the homogeneous width of hydrogen peroxide compared to water. This corresponds to a significant decrease in the decay time.

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POSSIBLE MECHANISMS OF CHANGING THE SHAPE OF ν_1 BAND OF METHANE AND DEUTEROMETHANE IN GASEOUS MIXTURES

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Physics of processes of relaxation of molecular excitations is one of actual problems of modern physical optics. Information on dynamics of the relaxation processes is necessary to clarify details of substance microstructure, particularly, the character of molecular processes in condensed state, for purposeful selection of active media of tunable lasers. Processes of molecular relaxation can be studied on the base of analysis of shape and parameters of band's contour in spectra of Raman scattering and IR absorption.

In this work we present results and discussion of possible vibrational relaxations with respect to formation of ν_1 band of methane and deuteromethane. Investigations of spectra of isotropic Raman scattering (IRS) were carried for pure methane (CH_4) and deuteromethane (CD_4), and its mixtures with Ar and Kr in gaseous phase within a wide interval of temperature and pressure.

In our experiment we observe that in all cases the contour of ν_1 band in gaseous phase at densities up to 10 amagat does not change its half-width, and at higher densities its half-width increases according to practically linear law.

We analyzed a series of mechanisms of the effect of broadening the IRS band ν_1 of full-symmetric vibrations. It was found to be that the main role in formation of the band's contour plays, obviously, the vibrational broadening. Vibrational relaxation plays a determining role in formation of contours of IRS bands of polyatomic molecules in condensed matters. Direct picosecond experiments with using the technique of stimulated Raman scattering and coherent active spectroscopy proved that the relaxation of phases of intramolecular vibrations of polyatomic molecules occurs much faster than the relaxation of population of proper vibrational levels. However, the observed quantitative difference between estimations and experimental results assumes that this mechanism is not the only one in the broadening effect.

In spite of the progress in understanding the processes of relaxation of vibrational excitations in condensed matters the problem is still actual one. It is appropriate to make an analysis of modern models of vibrational relaxation.

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ON MECHANISM OF NON-COINCIDENCE OF PARAMETERS OF STOKES AND ANTI-STOKES LINES IN A SPECTRUM OF RAMAN SCATTERING OF LIQUIDS

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According to current ideas on formation of width and shape of the contours of Raman scattering lines, frequencies of intramolecular vibrations must be coincident for Stokes and anti-Stokes components. Moreover, in polarization studies of the frequency of fundamental intramolecular vibration there must be the coincidence of polarized and depolarized components.

In [1] authors found a disturbance of these conditions. We studied Raman spectra in $CHCl_3$ and CCl_4 in Stokes and anti-Stokes regions.

	Stokes				anti-Stokes			
Substance	$\nu_\parallel$	$\nu_\perp$	$D\nu_\parallel$	$D\nu_\perp$	$\nu_\parallel$	$\nu_\perp$	$D\nu_\parallel$	$D\nu_\perp$
	in cm^{-1}				in cm^{-1}			
$CHCl_3$	260	258	8.3	10.4	365	366	8.8	9.2
	363	364	6.3	10.8	372	370	5.8	9.2
	668	667	6.4	7.3	671	670	5.9	7.3
CCl_4	215	216	11.2	11.2	220	221	9.5	11.3
	311	311	11.0	12.5	319	318	10.8	11.3

The observed behavior of parameters of Stokes and anti-Stokes lines in Raman spectra of liquids can be explained by a change of the energy structure of wave function of response (WFR) of molecules at transitions from one vibrational level to another [2]. The transition is accompanied by the change of the energy structure and, consequently, the frequency of WFR of molecules as a whole and of intramolecular vibrations.

The transition of molecule from the basic state to the vibrational one leads to weakening the energy structure of WFR of molecules, and it is accompanied by increase of the vibrational frequency of molecules as a whole, and, consequently, the frequency of intramolecular vibrations. Anti-Stokes component in Raman spectrum represents the excited level, where the frequency of molecules as a whole is higher than its magnitude in the basic state. Accordingly, the frequency of intramolecular vibrations in the excited state is higher than the frequency in the basic state that leads to the difference in frequencies of Stokes and anti-Stokes lines.

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VIBRATIONAL SPECTRA OF COMPLEXES WITH HYDROGEN BOND IN INERT SOLUTIONS

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We studied IR absorption spectra of hydrogen chloride and a series of proton donors with C-H groups in liquid argon, krypton, and xenon. As a proton acceptor we considered phosgene, acetone, dimethyl ether and acetonitrile. Solubility of these systems in inert solvents at low temperatures is studied.

Main attention was paid to study of spectral parameters of νHCl and C-H bands of proton donors in complexes of different acceptors with gradual change in proton-accepting ability of C=O and C≡N groups.

The absorption band of main vibration of HCl dissolved in liquid argon, krypton and xenon is of complicated shape, and it consists of two lateral P and R components and more or less intensive central Q component. Such a shape of the band is explained by rotation of molecule in the liquid. With rising activity of the solvent at transition from argon to krypton there is a rise of integral coefficients of absorption and the low-frequency shift of the band's mass-center. A narrow band $\Delta\nu_{1/2}$~10 sm^{-1} of $Cl_2CO\times\times\times H\text{-}Cl$ complex appears on the low-frequency wing of the band of hydrogen chloride.

In a typical complex of HCl with acetone there is a broad band of the complex with $\Delta\nu_{1/2}$~200 sm^{-1}. The low-frequency shift of the complex's band, as compared with a free molecule, is ~350 sm^{-1}. Formation of even weak complex leads to change of vibrational bands of the proton acceptor.

As C-H proton donor we used acetylene, methylacetylene and their deuteroderivatives. In this case also the rise of proton-accepting ability of proton acceptor leads to increase of the low-frequency shift of the band and its half-width. We carried out ab initio calculations of the energy of formation, vibration frequencies, dipole moments, and other parameters for the studied complexes. The calculations were performed in frames of HF-approximation with 6-31G(d, p) basis and total optimization of the geometry of molecules.

IR-SPECTROSCOPY AND THERMODYNAMICS OF ALKYLBENZOATES AND ALKYLHYDROXYBENZOATES: COMPARATIVE ANALYSIS

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Benzoates and hydroxybenzoates are widely used in various industries. Some of them act as food additives, drugs and stabilizing agents. All these properties are largely determined by the intermolecular interactions in condensed matter. The position and number of hydroxyl groups in the benzene ring also greatly affect the physical-chemical properties of hydroxybenzoates. For example, *para*-isomers of hydroxybenzoates or parabens under standard conditions are solids, and *ortho*-isomers or salicylates at the same conditions are fluids due to the inter- and intramolecular hydrogen bonds. In this regard benzoates and hydroxybenzoates are interesting objects for the study of intermolecular interactions and structure in condensed matter.

To study the effect of the structure on the intermolecular interactions of these compounds, we used the following physical methods: IR spectroscopy and solution calorimetry. IR spectroscopy was used to study the complexes of alkylhydroxybenzoates with proton acceptors in an inert solvent and the complex of alkylbenzoates with aliphatic alcohols. It was shown that parabenes forms strong intermolecular complexes and the strength of the hydrogen bond does not change in the homologous series (from methyl to butyl groups). In contrast, salicylates in solutions of proton acceptors doesn’t form hydrogen bonds with solvent due to the strong intramolecular hydrogen bond, which does not break even with strong proton acceptors as triethylamine. Also, it was found non-trivial fact, that alkylbenzoates (moderate proton acceptors) are not completely H-bonded in aliphatic alcohols. At the same time degree of complexation of these compounds in chloroform is 100 %. Analysis of IR-spectra shows, that strength of hydrogen bonds in complexes of benzoates with aliphatic alcohols and chloroform does not depend on the length of alkyl groups in the solute molecules.

By the solution calorimetry were measured thermal effects of dissolution of these substances in various proton donors and acceptors solvents [1]. Comparative analyses of spectroscopic and thermochemistry properties show a good correlation.

Employing these results, we have identified relation between of the structure and property of these compounds.

[1]. B.N. Solomonov, V.B. Novikov, M.A. Varfolomeev and N.M. Mileshko. J. Phys. Org. Chem. - 2005. - V. 18. -P. 49 - 61.

STUDY OF INTERMOLECULAR DYNAMICS OF CONDENSED STATES OF A MATTER BY ORIENTATION SPECTROSCOPY METHODS

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The depolarized components of molecular scattering of light (DCMSL) have been studied in liquids consisting of asymmetric-in-polarizability molecules within the wide range of temperature and frequency.

Toluene $C_6H_5CH_3$ and aniline $C_6H_5NH_2$ have been selected, their molecules have identical symmetry and the same base (benzene ring) but somewhat different chemical bonds. The results will be compared, which allows the effect of molecular structure on the scattering process to be revealed.

The studies have shown that the DCMSL contour observed for toluene and aniline (in the coordinates $1/\mathcal{J}$ and ω^2 where $\mathcal{J}$ is the spectral density of the DCMSL line contour) is a sum of the two dispersion ones within the range from 0 to 60 cm^{-1} with inflection about 20 cm^{-1} at room temperature. When the liquid is heated the inflection border shifts to low frequency.

The literature data on the far DCMSL spectra are very conflicting. We have scrutinized thoroughly the intensity distribution in far wings (60-200 cm^{-1}).

The statistical treatment of the wing shape by different analytical functions has shown that the best approximation is the Gaussian one. To explain this regularity we make use of Fisher's idea [1], the decreasing intensity of the far wings is considered as manifestation of dynamics of an initial collisionless mode of the time evolution of the scattering system. For the relaxation time ($\sim 10^{-13}$ s) the phase failure of some molecules forming a fluctuation occurs, which results in dephasing.

The behavior of the DCMSL spectra is discussed from the view point of hindered rotation of liquid molecules with taking into account the specifics of intermolecular interaction.

[1]. Fisher I.Z. JETF, 1981, 2, 540-549.

2D STUDY OF STRETCHING O-H VIBRATIONS IN THE PYRIDINE N-OXIDE/TRICHLOROACETIC ACID COMPLEX IN ACETINITRILE USING EXACT VIBRATIONAL HAMILTONIAN

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Recently, we performed calculations of 1D and 2D potential energy surface (PES) and frequencies of O-H vibrations in free title complex [1]. 3D calculations of PES and frequencies of O-H vibrations were performed in free title complex [2] and for complex in acetonitrile [3]. It was shown that the accuracy of calculations increases in the row 1D-3D. In particular, we note that the value of the O-H stret-ching vibration of the title complex in acetonitrile using 1D, 2D and 3 D calcula-tions were found 1070, 1041 and 1005 cm^{-1}, whereas the experimental value is close to 955 cm^{-1}. Carrying out these calculations, we used a somewhat simplified Hamiltonian and a set of Cartesian coordinates to describe the motion of the hydro-xyl hydrogen atom. In this work the exact 2D vibrational Hamiltonian for the Schrödinger equation of the form:

$$-F_{OH}\frac{\partial^2}{\partial q^2}\Psi - F_{OH}\frac{\partial^2}{\partial Q^2}\Psi - F_{OH}T(q)\frac{\partial}{\partial q}\Psi - F_{OH}T(Q)\frac{\partial}{\partial Q}\Psi - 2F_H\cos\theta\frac{\partial^2}{\partial q\partial Q}\Psi + U(q,Q)\Psi = E\Psi$$

was used. First of all the PES was calculated using and Q as stretching coordi-nates for O-H and O---H bonds in hydrogen bridge. Ranges of the coordinates changes were (-0.5 - +1,5 Å) and (-1- +2Å) respectively. Calculated in this way the hydroxyl group stretching vibration frequency was found to be 961 cm^{-1}, that is in the very good agreement with experimental one.

[1]. G. A. Pitsevich, A.E. Valevich, V. Sablinskas, I.U. Doroshenko, V.E. Pogorelov, V. Balevicius:. J. Spectrosc. Dyn. 2013, 3: 19

[2]. G. A. Pitsevich, A.E. Valevich, V. Sablinskas, I.U. Doroshenko, V.E. Pogorelov, E.N. Kozlovskya,V. Balevicius:.Vestnik of the Foundation for Fundamental Research, 2013, N1,p.80-87.

[3]. G. A. Pitsevich,O.V. Novichenok: in Abstracts of IV Congress of Belarusian Physicist,Minsk,2013,p.192.

LONG-WAVE SPRING TYPE VIBRATIONS IN THE RAMAN SPECTRA OF SOME NORMAL ALCOHOLS

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Intermolecular vibrations in hydrogen-bonded complexes in the gas, liquid and matrix isolation attracted the attention of researchers. However, the long-wave spectral range are still poorly understood. Often, the frequency range of 30-500 cm^{-1} is easier to obtain in the Raman spectra. On this basis, we recorded a number of long-wave Raman spectra of normal alcohols in the liquid phase (Fig.1)

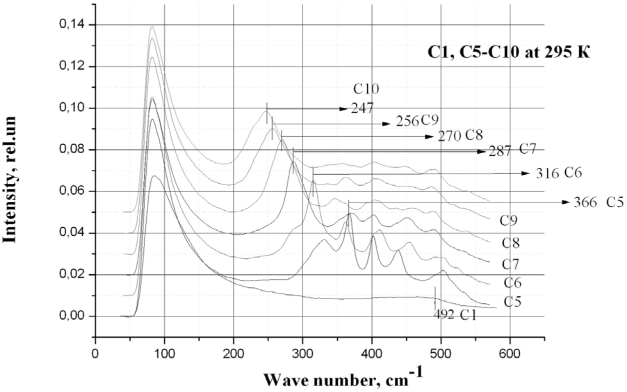

Figure 1. Long-wave Raman spectra of some normal alcohols.

As one can see from Fig.1 there is a monotonic shift to lower frequencies of the Raman lines in the spectral interval 400 - 200 cm^{-1} with increasing the size of alcohol molecules. We assumed that the investigated Raman lines are due to spring type vibrations when the length of the molecular skeleton increases and decreases due to expansion and contraction of the carbon chain due to synchronous changes of the C-C-C angles. To check this idea, using B3LYP/cc-pVDZ approximation we calculated the structure and Raman spectra of a series of normal alcohols. The calculated frequencies of the proposed type vibrations are in good agreement with the experimental data.

ESTIMATION OF SOLVENT EFFECTS ON N-H FREQUENCIES OF AMINES, OF ITS H-BOND COMPLEXES AND SELF-ASSOCIATIVE SPECIES BY IR-SPECTROSCOPY METHOD

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Intermolecular interactions significantly influence on properties of many supramolecular and biological systems. Intermolecular interactions influence on the characteristics of absorption spectrums. Today large quantity of models for estimation of influence of intermolecular interactions on IR frequencies is known.

In present study solvents effect on N-H stretching vibration frequencies of imidazole, pyrazole, pyrrole, pyrrolidine and methanol and its complexes with proton acceptors and proton donors were investigated. For analysis of solvent effects model [1] was applied. It is based on solvent parameter S_{VW}.

On the first stage absorbance of free molecules of imidazole, pyrazole, pyrrole, pyrrolidine were analyzed. It was shown that obtained N-H frequencies of these substances in proton acceptor and inert solvents linearly depend between them. Sensitivity to solvent is changed by next way pyrrole>imidazole>pyrazole>. It was shown that obtained N-H frequencies of these substances in inert solvents linearly on solvent parameter S_{VW}. Deviations in proton acceptors solvents from linear dependencies were induced by hydrogen bond formation.

In work frequencies of H-bonded N-H groups of pyrrol, imidazole, pyrazole in complexes with proton acceptors (N-H…B) in different solvents were obtained. In aprotic solvents frequency shifts were induced only by occurrence of van der Waals interactions. In proton donor environment ternary or more complicated complexes are formed. The strength of hydrogen bonds N-H…B in these complexes is changed due to cooperative effect.

Influence of solvent effects on self-association of pyrrole, imidazole, pyrazole in different solvents was studied. Formation of associative species induce occurrence of new N-H stretching vibration bands shifted to low frequencies. It was shown that increasing of polarity, proton acceptor and donor properties of solvents decreases degree of association. We propose a method for determining the enthalpy of self-association in the crystalline states. In order to confirm data were used method of van’t Hoff and Badger-Bauer rule.

[1]. Solomonov B.N., Varfolomeev M.A., Novikov V.B., Klimovitskii A.E. (2006) // Spectrochimica Acta A. V64**,** p.397.

THE EXCITATION SPECTRUM OF SINGLET OXYGEN AND PHOTOLUMINESCENCE OF METHYL PHEOPHORBIDE

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In many applications, including photodynamic therapy, efficiency of excitation of dye sensitizer to generate singlet oxygen ($^1O_2$) is assessed by the intensity of dye's visible photoluminescence (PL) because the direct detection of singlet oxygen is rather difficult.

We measured PM excitation spectra of PL bands of methyl pheophorbide (mPH (a)) at 730 nm and own emission of $^1O_2$ at 1270 nm under the same conditions of excitation with UV-Vis spectrophotometer Varian Cary 50(VC50). The PM excitation spectra of the (mPH (a)) was recorded using standard option of the VC50. To register an extremely faint $^1O_2$ own emission was used a specially designed detector, consisting of InGaAs cooled photodiode covered with a set of filters providing a narrow band of transmission centered at 1270 nm. Mentioned above detector was placed in the cuvette section of the VC50 directly next to the sample and was connected to the input of its own registration system independent of the VC50 intensity registration system but synchronized in time with scanning wavelength excitation of input monochromator of the VC50 spectrophotometer.

Comparison of the excitation spectra of $^1O_2$ emission at 1270 nm and PL of methyl pheophorbide (mPH(a)) schows that a choice of excitation of dye sensitizer to generate singlet oxygen ($^1O_2$) based only on assessment of dye sensitizer PL may be incorrect.

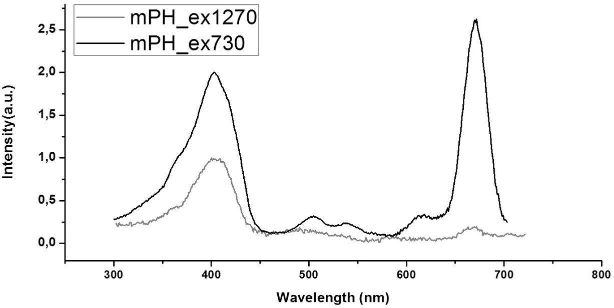

Figure 1. The excitation spectrum of singlet oxygen radiation and of photoluminescence of mPH(a) in chloroform

CONCOMITANT POLYMORPH MODIFICATIONS OF $C_{18}H_{17}F_3N_2O_4S$

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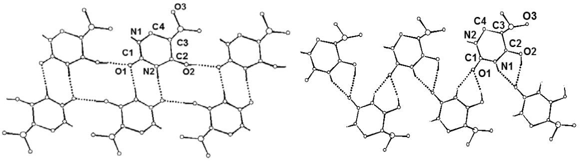
As a result of X-ray investigation recently synthesized $C_{18}H_{17}F_3N_2O_4S$ (I) [1] (new precursor for biologically active compounds) was found that this compound under identical conditions crystallized in the two polymorphic modifications: α (plate-shape, m.p. 208 ºC, d = 1.498 g×cm^{-3}) and β (prizm-shape, m.p. 226 ºC, d = 1.538 g×cm^{-3}). The main difference between α and β polymorphs is the type of intermolecular H-bonds pattern. The molecules of α by the quite strong intermolecular H-bonds are connected in centrosymmetric dimers which in turn are organized in 2D-net. In contrast to the α, the molecules of β by the system of the fork H-bonds form dimers, which are organized in 1D *zig-zag* chains. Parameters of H-bonds for α polymorph: N(2)-H···O(1) 2.969 Å, O(2)-H···O(1) 2.617 Å, N(2)HO(1) 163.1 º, O(2) HO(1) 170.6 º, for β polymorph: N(1)-H···O(1) 2.803 Å, O(2)-H···O(1) 2.823 Å, N(1)HO(1) 152.9 º, O(2)HO(1) 164.9 º. The molecules of α and β polymorphs has very similar molecular geometry, exept the slight difference of the core heterocycle N(1)N(2)C(1-4) conformation: the modificated parameters of the Cremer-Pople for α: S = 0.59, θ = 42.57 º, ψ = 7.52 º, conformation – *flattened half chair*, for β: S = 0.54, θ = 43.02 º, ψ = 27.42 º, conformation - *flattened half bath.*

The main peculiarities of H-bonding in α and β polymorphs of (I) were also characterized by the IR- and Raman spectroscopy.



Intermolecular H-bonds in α and β polymorphs.

[1]. Yu. G. Shermolovich, V. M. Timoshenko, et. all, Tetrahedron, in press.

FIELD-SUBSTANCE INTERACTION AND DIMENSIONAL EFFECT IN VIBRATIONAL SPECTRA

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According to [1], the energy density of the physical vacuum exceeds significantly the density of atomic nucleus. That is why structural-dynamic processes in condensed matters cannot be explained without taking into account the field-substance interaction. As a result of oscillating influence of the physical vacuum and surrounding particles an oscillating wave function of response (WFR) of particles is induced on a single molecule [2].

In IR absorption spectra of an out-plane vibration of benzene ν_{vib}=673 cm^{-1} a dependence of the intensity distribution within the absorption band on the amount of substance is observed (Fig.1). In the gaseous state the contour of the absorption band is represented by superposition of the central Q-branch and the lateral P- and R-branch ($\Delta\nu_{PR}$≈23 cm^{-1}). At the transition to the liquid state there is a transformation of the band, and at the layer thickness of about 3-4 μm the contour of the band represents the Q-branch with wide exponential wings (Fig.1a)

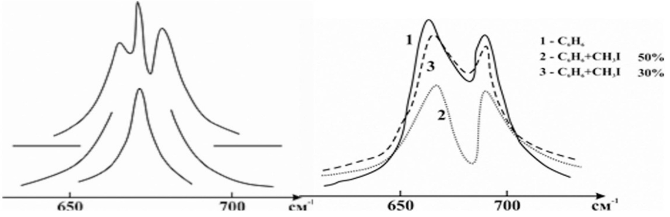

Fig.1. The contour of IR absorption band of benzene (ν_{max}=673 cm^{-1}): a – in the gaseous (1) and liquid (2) states (layer thickness ~ 3 μm), b – in the liquid state (1) and in solutions (2,3) at the layer thickness ~ 15 μm.

Increase of the thickness of the substance layer is accompanied by disappearance of the central Q-branch and imaginary restoration of P and R branches. The distance between intensity maxima of the lateral branches is rather equal to its magnitude in the gaseous state ($\Delta\nu_{PR}$≈23 cm^{-1}).

The absorption band with maximum at ν_{vib}=673 cm^{-1} belongs to the out-plane vibration of benzene. The central Q-branch is related to molecules involved in chaotic Brownian motion, and the lateral P and R branches are related to the energy structure of the self-coordinated field of molecules. At small thickness of the substance the WFRs of the Brownian molecules form the central Q-branch. With rising thickness of the layer there is an ordering of benzene molecules in the form of ~15 μm layers, as well as reduction of Brownian molecules.

[1]. Chernin A.D., Uspekhi Fiz. Nauk, v.171, p.1153 (2001).

[2]. Erkin N. Shermatov. Superconductivity and the memory of Man. – St. Petersburg: Izd. Polytechnic University, 2006. – 174 p.

QUANTITATIVE ANALYSIS OF INTRAMOLECULAR INTERACTION IN MOLECULES OF ARYLPOLYENES

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The interest to spectral and luminescent properties of arylpolyenes does not weaken about hundred years. Linear arylpolyenes thanks to the structure are of interest for spectrochemical researches and quantum chemistry calculations of electronic conditions, and also have wide practical application. Interpretation of electronic spectra of the investigated molecules with unbranched π-electron system, to reference of observable strips to the separate electron-vibrational transitions, spent on the basis of the display account in spectra intra- and intermolecular interactions, supplies the valuable information on a structure and properties of molecules.

Strong electron-phonon interaction in investigated molecules is shown in the big width and considerable intensity a phonon wing (PW). Which together with a zero-phonon line (ZPL) makes the vibronic bands. Set PW creates intensive enough background on which peaks of thin structure are located.

The spectra of four arylpolyenes are modeled by representing the band of each of the vibronic transitions as the sum of a ZPL and a PW with certain parameters (half-widths, Debye-Waller factors)[1]. The spectra calculated in this fashion coincide with the experimental spectra. This makes it possible to determine the relative intensities of vibronic transitions. Calculation and the comparative analysis of parameters of intramolecular interactions forming fine-structure fluorescence and fluorescence excitation spectra of four investigated molecules is carried out. Revealed the anharmonicity in the spectra of fluorescence and fluorescence excitation is explained by an interference of the Franck-Condon and Herzberg-Teller interactions

[1]. Naumova N.L., Vasil’eva I.A., Osad’ko I.S., Naumov A.N. Jornal of Luminescence, 2005, v.111, p.37-45.

NMR, FTIR AND X-RAY DIFFRACTION STUDIES OF PROTON TRANSFER PATHWAY IN SHORT- AND VERY SHORT H-BONDS

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Developments in the hydrogen bond (H-bond) research show persisting or even boosting interest in this type of interaction having a great importance in many physical or chemical processes. Because of its abundance and importance in the molecular world and beyond precise definition of H-bond, detection and evaluation of energy, determination of proton transfer pathways and monitoring of proton dynamics are subjects to continuous debate and research [1].

The H-bonded complexes of pyridine N-oxide (PyO) with H_2O, acetic, cyanoacetic, propiolic, tribromoacetic, trichloroacetic, trifluoroacetic, hydrochloric and methanesulfonic acids have been studied by FTIR and ^{1}H, ^{13C} and ^{17}O NMR spectroscopy, X-ray diffraction and quantum chemical DFT calculations.

Correlations between NMR chemical shits, vibrational frequencies of the NO stretching and PyO ring modes and geometric parameters of the H-bond have been established. The experiments show and DFT calculations confirm that definite discontinuity is present in the vicinity of the midpoint in the proton transfer pathway.

The established correlations significantly aid understanding of fine effects such as the isotope (deuteration) effect, crystal-to-solution transition, criticality of aqueous solutions induced by ionic pairs or molecular processes in nano- and mezo-scales [2].

[1]. Book of abstracts of XIX. International Conference on "Horizons in Hydrogen Bond Research", September 12-17, 2011, Göttingen, Germany, http://www.hbond.de

[2]. V. Balevicius, K. Aidas, I. Svoboda and H. Fuess, J. Phys. Chem. A 116, 8753 (2012).

EFFECT OF ENVIRONMENT ON ENERGY STRUCTURE OF EMISSION CENTERS IN SOLUTIONS WITH COPPER IMPURITY

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The investigation of energy structure of a copper ion impurity ($10^{-3} – 10^{-1}$ mol/l) in aqueous solutions of oxygen-containing salts and acids is presented.

It was found that at very low values of an activator ion (copper) impurity concentration C_x the luminescence intensity in our materials is proportional to the activator concentration C_x.

The absorption, luminescence, luminescence excitation spectra of a copper impurity in the frozen aqueous solutions H_2SO_4 , $HClO_4$, Na_2SO_3 , Na_2SO_4 were studied in the temperature range of 77–290 K. Those solid solutions are characterized by three types of bands of absorption and emission.

The effect of alkali-haloid salt cations on the absorption, luminescence, luminescence excitation spectra in the solutions with copper ion impurity was elucidated. Those cations influence electrostatically on copper complexes in given solutions.

Experimental results obtained are interpreted on the basis of an ionic model for complexes in the solutions under study. The long-wave emission band can be ascribed to the $d^9s \rightarrow d^{10}$ transitions in a free Cu^+ ion.

TEMPERATURE EVOLUTION OF CLUSTER STRUCTURES IN 1-HEXANOL AND 1-OCTANOL

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The alcohols belong to the specific kind of species since their molecules can form hydrogen bonds and arrange in different structures named clusters. The dependence of FTIR spectrum of pure 1-hexanol and 1-octanol on the temperature was investigated. The measurements were performed for frozen (the minimum temperature −150°C) and liquid phases of both alcohols (the maximum temperature 40°C). All changes in IR spectrum of investigated species during gradual warming were detected and analyzed. On the bases of preset observations, the conclusions concerning the evolution of cluster structures in 1-hexanol and 1-octanol during transition from solid (frozen) state to liquid state were made. These assumptions were confirmed by ib initio calculations of energy parameters and IR spectra of considering cluster structures.

Acknowledgment

This work was made with supporting of DFFD (Derzhavnyi Fond Fundamental’nyh Doslidzhen’).

SPECTRAL AND PHOTOPHYSICAL PROPERTIES OF ACTIVE ELEMENTS BASED ON LASER DYES IN ALIPHATIC POLYURETHANE MATRIX

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Dye lasers are widely used as a coherent light source in spectroscopy, nonlinear optics, medicine, and lidar technology. Stable operating time of dye lasers depends on the chosen components of active media, namely, polymer matrices and dyes. Polymer matrix should provide sufficient beam strength, transparency, high solubility of dyes, and dye stability during storage and operation.

In this study, a new polymer matrix based on aliphatic polyurethane was proposed and investigated for the development of laser active media for the tunable dye lasers. The polymer matrix was synthesized by the prepolymer method. The prepolymer, obtained from hexamethylene diisocyanate and oligodiethyleneglycol adipinate, was hardened by trimethylolpropane. Well-studied polyurethane acrylate, obtained by photoinduced (benzoin isobutyl ester is a photoinducer) radical polymerization of oligourethane acrylate was used as a matrix for a comparison.

The production method of the laser triplexes (glass – polymer – glass) active media based on xanthene and pyrromethene dyes was described, their spectral, photophysical and generation characteristics were investigated. Significant increase in the beam strength of the polymer matrix, the growth in efficiency and stability of the active elements were observed due to the peculiarities of aliphatic polyurethane chemical structure. The main reason for the high photostability and operation lifetime of laser polyurethane-based active elements was shown to be the absence of reactive radicals.

Formation of covalent and hydrogen bonds between aliphatic polyurethane matrix and coumarine or phenalenone dyes was investigated by means of IR-spectroscopy method.

PROBING OF HIGHER EXCITED STATES OF DYE MOLECULES BY ANISOTROPY EXCITATION SPECTRA

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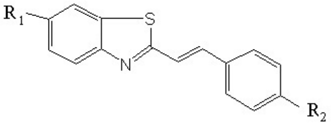
High-intensity laser radiation and high-energy photons are widely used to excite the molecules in addressing a variety of research and applications in optics, chemical physics, quantum electronics, biophysics and other fields of science. Under such influences on substance the significant part of absorbed energy will inevitably be transformed by high electronically excited states (HES) of molecules. Particularly noteworthy phenomenon involving HES of polyatomic molecules populated by non-linear photoexcitation. The fundamental importance of the nonlinear excitation is a molecule that can pass significant energy and selectively convert it to a given quantum state. The rationale for the relevance of the study of processes involving HES molecules are real perspectives of the results obtained when design the element basis of optoelectronics, development of fluorescent probes and sensors the read methods and input signals into complex biopolymer structures in optical recording media, design of lasers on organic compounds, in modern biomedical technologies.



In this work the results of study of the electronic properties of new specially synthesized neutral basis of styryl dyes with different terminal groups. Spectral properties of the substances were studied in liquid acetoniyrile, ethanol and high viscosity glycol solutions at room temperature.

Optical absorption spectra of solutions were recorded using a Specord UV VIS spectrophotometer. Fluorescence emission and excitation spectra were recorded by Carry Eclipse e Fluorescence Spectrophotometer.

Quantum-chemical calculations were performed with the goal of understanding the features of the electron density distribution in the ground and excited states as well as the changes in the molecular geometry of dyes under excitation to explain the maximum anisotropy values experimentally measured.

We demonstrate an experimental technique which relies on the orientation of the excited-state absorption transition dipole moments $S_1 \rightarrow S_n$ (n = 2,3, 4...) to determine the spectral position and orientation of the transition dipole moments connected with the $S_0 \rightarrow S_n$ transitions (n = 1,2,3...). Based on the experimental and calculated results we use an approach for the investigation of the anisotropy properties of linear polymethine molecules, which can be applied to cases in which the steady-state measurements cannot be used because of too low intensity of the corresponding spectral band.

4

CRYSTALS

THERMAL AND OPTICAL PROPERTIES OF MOLECULAR CRYSTALS WITH SELF-ORGANIZING DISORDER

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Disordered molecular solids in particular structural and orientational glasses, glassy crystals, crystals with a partial orientational ordering, metastable polymorphs and other more complex systems, form a broad class of solids exhibiting new physical phenomena concerned with physics of disordered systems. The goal of this study was to investigate experimentally thermal conductivity and low-frequency Raman spectra [1] of simple molecular systems, orientational glasses in the temperature region 2-150 K. The objects were molecular orientational glasses (ethanol (C_2H_5OH), freon 112 ($C_2F_2Cl_4$), freon 113 $C_2Cl_3F_{3,}$ cyanocyclohexane ($C_6H_{11}CN$), cyclohexanol ($C_6H_{11}OH$) and cyclohexene (C_6H_{10})). The main emphasis is here focused on the influence of the conformational disorder upon the different properties of this material. It is found information about the existence of optical phonons contributing to the heat transport orientational glasses. The thermal conductivity contribution from optical phonons strongly depends on the geometrical details of the unit cell of the particular crystal.

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POLAR VIBRATION CLASSIFICATION AS SOURCES OF NEGATIVE DIELECTRIC PROPERTIES IN CRYSTALS

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Simplified model without damping ($\Gamma = 0$) based on the well-known Kurosawa ratio gives the negative frequency region of dielectric permittivity (DP) between the transverse ω_T and longitudinal ω_L phonons frequencies (T – L splitting). Indeed, within this approximation $\varepsilon(\omega)\rightarrow-\infty$ at $\omega\rightarrow\omega_T$, for any frequencies pair $\omega_T < \omega < \omega_L$. However, in the case when damping is present ($\Gamma >> 0$), the real part of DP cannot reach negative values. The effect of damping the polar vibrations on dispersive properties of the crystalline media has been studied in this work. It has been shown that just the damping action plays a principal role both in shaping of the minimum achievable negative value of DP and width of the frequency area of its existence.

Our analysis shows that a large number of crystals with one pronounced vibration in the infrared region, such as classic items of alkali-halide crystals (NaCl, KBr, NaF, LiF, and many others) in the anomalous dispersion region reach sufficiently high in modulus negative values of DP. For these crystals, the difference $\omega_L - \omega_T$ reached tens of THz, whereas the damping constant Γ was typically less than one THz at room and low temperatures. Therefore, the ratio $\Gamma/(\omega_L - \omega_T) < 0.1$ ensures the existence of high in modulus negative values of DP observed in practice. Moreover the frequencies range with $\varepsilon'(\omega) < 0$ almost coincides with the interval of T – L splitting in this case. However, the absence of negative DP with relative damping $\Gamma/(\omega_L - \omega_T)>1$ has been recently found by us in a lot of crystalline media.

Presented (in full report) our analytical dependences between the main parameters of crystals may be the basis for polar vibration classification as sources of negative dielectric properties in crystalline media with rather complicated phonon spectrum.

ELECTRONIC SPECTRA AND PROPERTIES OF NOVEL LAYERED SUPERCONDUCTORS

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The discoveries of superconductivity in transition-metal borocarbides RNi_2B_2C (R=Y, Ho, Er, Tm or Lu) and RFe_4Al_8 aluminides have initiated extensive studies of their physical properties. Another Fe-based superconductors – pnictides and chalcogenides - recently attracted a great interest due to larger transition temperatures. These systems show a variety of properties, including exotic magnetic behavior and coexistence of magnetism and superconductivity. The relative structural simplicity and anisotropy of these compounds favor experimental and theoretical studies of chemical substitution and high pressure effects, both uniform and uniaxial. These studies are aimed at understanding of elusive mechanism of the superconductivity in these compounds, which contain magnetic 3d atoms.

This work presents a theoretical study of electronic structure and magnetic properties of RNi_2B_2C, RFe_4Al_8, and $FeSe_{1-x}Te_x$. The electronic structure, magnetic moments and susceptibilities were calculated ab initio within the local spin density approximation of the density functional theory. The calculations of the electronic density of states (DOS) show that the Fermi energy E_F is located close to pronounced peaks of DOS. The main contribution to the density of states at the Fermi level arises from the 3d electrons. The calculations of pressure dependent electronic structure and magnetic susceptibility in the normal state indicate that the novel superconductors FeSe and FeTe are very close to magnetic instability with dominating spin paramagnetism. It is shown that experimental data on pressure dependence of the superconducting transition temperatures in FeSe and RNi_2B_2C correlate qualitatively with the calculated behavior of DOS(E_F) with pressure.

EVIDENCE FOR NEW TYPE OF MAGNETIC EXCTATIONS IN FERROBORATE $NdFe_3(BO_3)_4$

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This report presents the results of resonance studies for a trigonal antiferromagnet $NdFe_3(BO_3)_4$ in which established a strong correlation between the dielectric constant, the electric polarization, magnetostriction and the magnetic state.

In the compound a sequence of magnetic phase transitions are observed. Below the Neel temperature T_N= 30.6 K exist an antiferromagnetic ordering of the magnetic subsystem of iron. This magnetic ordering induces magnetostriction and a weak spontaneous polarization in the plane ***ab*** which linearly increases with temperature decreasing The spontaneous polarization can be associated with the occurrence of an additional anisotropy in the plane ***ab*** induced by mechanical stresses due to the magnetoelastic interaction.

At the temperature T_c= 10.5 K another phase transition accompanied by a helicoidal incommensurate magnetic structure along an axis perpendicular to the light plane ***ab*** is observed**.** Anisotropy in this plane leads to a nonlinear deformation of the structure, which can be interpreted as a transition to a quasi-soliton structure. Finally, at lower temperatures, apparently occurs magnetic ordering of Nd subsystem.

In the study of the frequency dependence of quazi-ferromagnetic AFMR branches of $NdFe_3(BO_3)_4$ in the frequency range 27 - 32.2 GHz an additional absorption associated with the formation of an incommensurate magnetic superstructure is found. A characteristic feature of this exitaion is splitting of the absorption band into two parts: one of which is a further and tends to gap $\Delta\nu$ = 27.58 GHz in zero magnetic field, the resonance field of the other increases.

LOW-ENERGY VIBRATION SPECTRUM OF THE CRYSTAL $CsDy(MoO_4)_2$

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The crystal $CsDy(MoO_4)_2$ belongs to a series of rare-earth compounds in which the low-temperature phase transitions caused by the cooperative Jahn-Teller effect are observed [1]. Such compounds are interested as laser materials [2] and low dimensional magnetic structure materials [3]. It is necessary to know the structure of low-frequency vibration and electronic spectrum for predicting the physical properties of these materials at low temperatures.

$CsDy(MoO_4)_2$ has an monoclinic crystallographic structure at temperatures above 120 K, orthorhombic structure (Pcca, Z=2) at temperatures 120÷40 K and monoclinic structure ($P2_1/c$, Z=4) at temperatures below 40 K [4]. The transmission spectra of $CsDy(MoO_4)_2$ single crystals in the far IR region (13–100 cm^{-1}) in polarized light (**E**||**b**, **E**||**c**, where **b** and **c** are crystallographic axes) at a temperatures T=6÷40 K were studied previously [5]. The compound has a layered crystal structure, which is formed by layers of Cs^+ ions with weak bonds and layer packets $Dy(MoO_4)_2^-$ with stronger bonds. The low-frequency phonon spectrum is determined by interlayer vibrations. This allows applying one-dimensional model [6] for calculating low-frequency phonon spectrum at the temperatures below 120 K. We use frequencies obtained experimentally to calculate the shear force constants and to plot dependences of the vibration mode energies upon the wave vector.

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TERAHERTZ SPECTROSCOPY OF MULTIFERROIC IRON BORATES

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Iron borates with the general formula $R\mathrm{Fe}_3(\mathrm{BO}_3)_4$ (R= Y, La-Lu) crystallize in a trigonal structure of the natural mineral huntite, SG *R32*. Some of them undergo a structural phase transition into the $P3_121$ low-temperature phase. All these crystals order antiferromagnetically at temperatures T_N of about 40 K, demonstrate the magneto(di)electric effects, and belong to a new class of multiferroics. which promises device applications because magnetic properties can be governed by an electric field and vice versa.

My group carries out systematic optical studies of rare earth (RE) iron borates. In this talk, I'll consider recent terahertz spectroscopy results on europium [1], praseodymium, neodymium, and samarium compounds. The spectra of $\mathrm{EuFe}_3(\mathrm{BO}_3)_4$ present a clear evidence of a first-order structural phase transition at T_S = 58 K. This transition manifests itself by sharp shifts of phonon frequencies and by a sudden appearance of new vibrational modes. Peculiarities at T_N observed in the phonon frequency vs temperature curves manifest a spin-lattice coupling. The mechanism of this coupling is, most probably, connected with atomic displacements stimulated by the internal magnetic field arising in the magnetically ordered state below T_N. Similar peculiarities at T_N were observed in the spectra of other studied iron borates. For the Nd and Pr compounds, manifestations of an interaction between the lattice phonons and the crystal-field levels of the RE^{3+} ions were observed.

I am grateful to my coauthors of Ref. 1. A financial support of the Russian Academy of Sciences under the Programs for basic research is acknowledged.

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PLASTIC DEFORMATION OF DIAMONDLIKE CRYSTALS AT ROOM TEMPERATURE

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It has not yet managed to obtain mobile dislocations of large diameter at temperatures below 1400^{0}C on diamonds. The dislocations were introduced by pricking the diamond surface {001} with metal covering using microhardness tester with Vikkers indenter at room temperature. Loading on the indenter was 500 - 900 G, loading time was 10 - 60 sec.

Most expressly the effect of plasticity was shown at applying the perfect, blank coverings. In our case, for Cr and Al coverings applied by resistive deposit method, Al coverings have appeared the best. Cr coverings had breaks and cracks that had negative impact on the effect of plasticization. In the case of coverings applying by gas-transport method, the coverings turned out to be much better than at the resistive method, but the surface of the diamond monocrystal spoiled that had its negative effect as well. At the same time we did not observe any essential effect of coverings adhesion.

Great external pressure, which we use at diamonds samples indentation, creates a number of dislocations in plastic coverings. This dislocations move at high velocity. And as it is known the increase in velocity of dislocations when its kinetic energy reaches the height of power barriers causes dragging of dislocations which has dynamic character and is limited by transfer of energy from the dislocations to various elementary of excitation in crystals (phonons, magnons, electrons, etc.).

Having analyzed dragging mechanisms of dislocations moving at high speeds, we can assume that dislocations formation in plastic covering under high external pressure leads to the local phonons excitation, that is to local warming up of the material in the indentation area. It is known that diamond has high heat conductivity. Therefore heat from the covering is easily transmitted to the diamond, and the dislocations formation occurs in normal conditions for the given material, and not in the region of fragile destruction.

EXAFS STUDY OF NICKEL PHTHALOCYANINE DOPED BY KALIUM

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Magnetic properties of compounds are ususally originated of localized d- and f-electronic states of metal ions. Recently a new class of magnetic materials was revealed, where noncompensated spin magnetic moment is formed by p-electrons of nonmetal atom [1, 2]. Application of these materials is drastically limited by weak spin coupling so that magnetic order vanishes at tempetare of several dozens Kelvin, and, in most cases, compounds are antiferromagnets.

In this work Nickel Phthalocyanine (NiPc) doped by Klaium was studied, as a potential Room-temperature ferromagnet with molecular origin of its magnetizm [3]. The local atomic structure of Nickel was studied by Extented X-Ray Absorbtion Fine Structure (EXAFS) spectroscopy and complimetary theoretical analysis of spin properties was performed within density functional theory.

The EXAFS study revealed unchanged NiPc molecules together with Nickel clusters, which should not influence magnetic properties due to small concentration of metallic Nickel.

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TEMPERATURE EFFECT ON LUMINESCENCE FROM RADIATION-INDUCED DEFECTS IN SOLID KRYPTON

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Electronically-induced defect formation essentially renormalizes the luminescence spectra of rare-gas solids. Point defect formation under selective excitation of excitons in rare-gas solids by photons with energies $h\nu < E_g$ results in accumulation of Frenkel-pairs by intrinsic excited-state mechanism of defect formation via self-trapping of excitons [1]. Recently the simple kinetic model was proposed, which allows fitting the experimental dose dependences of "defect" luminescence subbands and obtaining the particular kinetic parameters [2]. At the same time it is well known that there is a strong thermal quenching of the defect formation processes in rare-gas solids, which was initially explained by temperature dependence of lifetime of emitting states. In the present study we apply the Eyring's transition state concept to the processes of thermal activation-inactivation of exciton trapping states in solid Kr resulting in luminescence spectra evolution under selective synchrotron irradiation.

The photoluminescence experiments were carried out at the SUPERLUMI-station at HASYLAB, DESY, Hamburg [3]. The dose dependences of luminescence of self-trapped excitons at different temperatures under irradiation by photons with energies $E < E_g$ were measured. These curves are saturated at long time of irradiation therefore we used the slopes of the initial linear parts of the dose curves at $t = 0$ as the defect formation rates w. Following Eyring assumption we can fit the temperature dependence of the defect formation rate by formula $w(T) = \beta \cdot T \cdot \exp(-E/kT) \cdot (1 + \exp(\Delta S/k) \cdot \exp(\Delta H/kT))^{-1}$. Here k – the Boltzmann's constant, E – Arrhenius activation energy, β – scaling factor. The values of activation energy E and enthalpy of inactivation ΔH may be determined from the upper and lower tangents of the $w(T)$ in the coordinates $(\ln[w(T)])$ vs. (T^{-1}). The value of entropy of inactivation ΔS may be obtained from the equilibration condition $d(\ln[w(T_{max})])/dT = 0$. The best fit of the data is obtained with $T_{max} = 27$ K, $E = 4$ meV, $\Delta H = 30$ meV, $\Delta S = 1$ meV·K^{-1}. The similar effect was observed for solid Xe and evaluation of the data is in progress.

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ELECTRONIC STRUCTURE AND ORIGIN OF LUMINESCENCE OF $K_2BiZr(PO_4)_3$ CRYSTALS

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Phosphates of alkali and four-valent cations are intensively studied as perspective luminescent materials. In particular, Zr^{4+}- and Bi^{3+}-containing phosphate crystals have attracted attention due to their applications as luminescent materials and hosts for luminescent ions. However at present, there is a considerable lack of scientific data about the nature of intrinsic emission and peculiarities of the excitation energy relaxation in these compounds. Complex analysis of the photoluminescence (PL), PL excitation spectra and reflectance spectra together with result of theoretical calculation are very useful for this task.

Polycrystalline samples $K_2BiZr(PO_4)_3$ were synthesized by spontaneous crystallization method.

Luminescence properties under VUV-excitation were studied in 3.7–20 eV region of excitations energies in 10-300 K temperature range on SUPERLUMI station (HASYLAB (DESY) Hamburg, Germany. Dependencies of luminescence intensities and peaks maxima position on temperature were obtained for different synchrotron radiation excitation wavelength. Luminescence spectra for excitation with N_2-laser (λ_{exc}=337nm) radiation also were obtained. Diffuse reflectance spectra of fine-grained powdered samples were measured at 300 K using double beam VUV spectrophotometer. The electronic structure calculations were performed by full-potential linear-augmented-plane-wave (FLAPW) method [1].

Luminescence spectra of the $K_2BiZr(PO_4)_3$ consist of few overlapping bands in 280 - 700 nm spectral region. Excitation spectra of these components significantly differ each other. In addition, short-wavelength emission band reveals nanosecond decay component under excitation in UV region while long-wavelength band – only microsecond components.

Luminescence emission and excitation spectra and calculated electronic structure of the $K_2BiZr(PO_4)_3$ were compared with corresponding properties of the $KZr_2(PO_4)_3$ and ZrP_2O_7 crystals. Origin of intrinsic luminescence and structure-related properties are discussed.

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LOW-TEMPERATURE ELECTRON SPECTRA FEATURES OF IMPURITY NAPHTHALENE CRYSTALS

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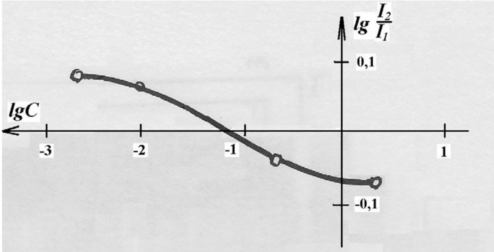
In most cases the presence of two band systems is a characteristic feature of absorption and emission spectra for impurity molecular crystals: series of narrow line bands (part of them with a multiplet structure) and series of structureless bands which positions, forms and intensities depend appreciably on temperature and impurity contents. In this work we present the results of a study aimed at the determination of the nature of both types of spectra.

The low-temperature absorption and fluorescence spectra of fluoronaphthalene in crystalline naphthalene were studied at various impurity concentrations. A doublet structure of impurity centers with the initial bands ν_{01}=31322 cm^{-1} (centre I) and ν_{02}=31226 cm^{-1} (centre II) which resonantly coincide with the corresponding bands in fluorescence spectra is clearly observed in the absorbance spectra. The doublet structure in these spectra may be explained on the basis of symmetry characteristics of the crystal and the impurity molecule.

The analysis of the absorbance spectra has allowed us to establish that the fractions of impurity centers of types I and II depend on impurity content (fig. 1). When the impurity content increases to about 1 wt. % a new structure appears in the spectrum: for each center a band against the wide structureless background emerges at the short-wavelength side of the bands at the distance of 45 cm^{-1}. At the same time a number of doublet bands emerge at the long-wavelength side of the center II band in the fluorescence spectra.



The obtained results have been discussed on the basis of a possible formation of as solid solutions of the substitutional type as interblock solutions and also generation of aggregate centers consisted of some impurity molecules with closely spaced energy levels that interact with each other as the impurity content increases. The observed transformations in the spectra may be due to the above mentioned reasons.

ON POLYMORPHISM OF TRIPHENYL PHOSPHITE

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The glass-former triphenyl phosphite (TPP) has been intensively studied since the discovery [1] of a new apparently amorphous state, called the ‘glacial’ state that is different from the glass and the normal crystal. The existence of more than one amorphous phase for TPP has been called ‘polyamorphism’ phenomenon. This unusual phenomenon stimulates intensive experimental research [2-4]. However, in this paper, for the first time we provide experimental evidence indicating that TPP can exist under two different crystalline phases.

IR spectroscopy was applied to identify the crystalline phases, and differential scanning calorimetry was applied to follow the thermodynamic evolution of the different phases versus temperature. Results presented here show that, in addition to the already known conventional crystalline phase, which melts at 300 K, TPP can crystallize in another polymorphic phase. The new polymorph was obtained from the liquid phase due to direct cooling from the room temperature up to 240 K where it is held for 15 min. The temperature was then increased up to 270 K where the continuous transformation of the supercooled liquid into the crystal was investigated. The new phase being metastable melts below the conventional one, i.e. at 291.7 K.

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ORIGIN OF THE DYNAMIC CROSSOVER IN THE GLASS FORMER ORTOTERPHENYL

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We have conducted infrared spectroscopy and differential scanning calorimetry measurements on ortoterphenyl (OTP) between 104 K and 333 K, aiming to explore the physical nature of the dynamic crossover at 1.2*Tg* found in variety experiments on OTP [1-3].

Results presented here show that in the region of the crossover temperature ~ 290 K (~1.2*Tg*) in the supercooled liquid OTP the crystal nuclei appeared. The appearance of the nuclei would change the molecular dynamics from individual to cooperative at $T<1.2Tg$, in other words would lead to spatially heterogeneous dynamics reported in [1-3]. Our results suggest that the origin of the dynamic crossover temperature near *Tg* is related to the formation of the fluctuating nuclei as the temperature ~ 1.2*Tg* is approached.

Taking into account our previous studies of salol, benzophenone and 2-biphenylmethanol we can conclude that the existence of nucleation near *Tg* is a universal feature of molecular glass formers.

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INVESTIGATION OF MAGNETIC PHASE TRANSITION IN $LiCoPO_4$ SINGLE CRYSTAL BY RAMAN SCATTERING

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The Raman scattering due to magnons and electronic excitations was measured in single crystals of $LiCoPO_4$ in the antiferromagnetic and paramagnetic phases ($T_N = 21.7$ K). Crystal field theory shows, that the Co^{2+} ion have six doubly-degenerate low-lying energy levels with a total splitting of about 0 – 1700 cm^{-1} [1]. The main attention was focused on the excitations of the magnetic phase coming from the 3 lowest doublets (0 – 1200 cm^{-1}). The experimentally detected energies in the paramagnetic state of electron excitations were found in regions at 200, 590 and 990 cm^{-1}. Strong coupling between these excitations and optical phonons was observed. The Raman scattering spectra are temperature dependent and they show the different changes at $T < T_N$, such as: appearance of additional lines and energy shifts of electron excitations. The anisotropy and exchange fields due to the antiferromagnetic ordering lift the Kramers degeneracy of Co^{2+} electronic levels. Excitonic states, which are formed in the atniferomagnetic phase, were observed. Besides, interaction between the magnetic sublattices can result in Davidov splitting of excitonic levels. The new lines at 39 and 46 cm^{-1} (at 5 K) were assigned to magnons. The intensity of these lines decreases with increasing temperature and the lines vanish above T_N eventually. The values of their energies are in agreement with result of inelastic neutron scattering measurement, namely, 37.9 ± 1.9 cm^{-1} (4.7 ± 0.24 meV at 8 K) [2].

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LATTICE VIBRATIONS AND STABILITY OF AlF_3

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The first-principle calculations are employed to study lattice dynamics of aluminium fluoride. The equilibrium stuctures of cubic and rhombohedral lattices and lattice vibrations were calculated within the density functional theory using CRYSTAL06 program. Phonon frequencies were calculated in the symmetric directions Γ-X, Γ -M and Γ -R of the Brillouin zone using different supercells. The phonon dispersion curves show large instability region around M-R direction. The largest phonon instabilitie occured at the R point of the Brillouin zone causing rhombohedral deformation of crystal lattice.

STRUCTURE EFFECT ON MOLECULAR DYNAMICS AND THERMOTHROPIC PROPERTIES OF CATANIONIC SURFACTANTS STUDIED BY FTIR SPECTROSCOPY AND DSC ANALYSIS

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Recently, binary mixtures of oppositely charged cationic and anionic surfactants, so called catanionic surfactants (CAS), are attracting a lot of interest due to their remarkable ability to form a variety of self-assembled structures both on solid surface and in air-water interface, and are of great application potential in nanotechnology for synthesis of various nanoobjects, as well as for various encapsulation and controlled-delivery processes in pharmacy, medicine, and biology. It was found that the phase transition pattern in CAS depends on many factors, therefore there is a need to investigate solid state CAS structure, thermal properties and phase behavior in more detail. In the present research, we report on the structure and molecular dynamics of solid phase complexes of a cationic surfactant cetyltrimethylammonium bromide (CTAB), $[H_3C\text{-}(CH_2)_{15}\text{-}N^+(CH_3)_3]^+Br^-$, with stearic acid ($H_3C\text{-}(CH_2)_{16}\text{-}COOH$, SA) as an anionic surfactant. Several bulk concentrations of CTAB were employed ranging from 0.2 to 0.8. The prepared complexes were characterized using FTIR spectroscopy and DSC analysis. It was shown that mixing CTAB with SA results in a formation of novel CAS compound comprising both SA and CTAB tails. Upon heating, a series of phase transitions occur, yielding finally an orientationally disordered hexagonal structure. The structural effects on the phase diagram and molecular dynamics of SA-CTAB aggregates are discussed.

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LUMINESCENCE SPECTROSCOPY, ELECTRONIC STRUCTURE AND ORIGIN OF LUMINESCENCE IN Bi-CONTAINING PHOSPHATES AND MOLYBDATES

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The bismuth and alkali metal phosphates/molybdates both undoped and doped with luminescent ions have attracted much attention last decade due to their applications as effective components for white light emission diodes and laser materials [1]. Clarification of the origin of intrinsic luminescence processes is an indispensable condition for elaboration of effective luminophores on the base of Bi-containing phosphates and molybdates.

In this work, the origin of intrinsic and dopant-related luminescence in the set of Bi-containing phosphate and molybdate crystals is studied by computational and experimental methods. The polycrystalline samples of undoped and RE-doped $BiPO_4$, $K_3Bi_5(PO_4)_6$, $K_2Bi(PO_4)(MoO_4)$, $K_2Bi(PO_4)(WO_4)$ and $K_5Bi(MoO_4)_4$, (RE = Eu, Tb, Pr, Tm, Ce) are synthesized and studied by the spectroscopic methods. The photoluminescence (PL) spectroscopy studies were carried out under the VUV (λ_{exc} = 90 – 333 nm, SUPERLUMI station at HASYLAB (DESY), Hamburg, Germany) and the N_2-laser (λ_{exc} =337.1nm) excitations in 4.2 – 300 K temperature region. The electronic band structures of undoped crystals were calculated by the FP-LAPW method [2]. Diffuse reflectance spectra of fine-grained powdered samples were measured at 300 K using double-beam spectrophotometer.

At the liquid helium temperature, all studied compounds reveal complex bands of intrinsic emission (quenched below 300 K) which comprise at least two components with peak positions in the red and blue-violet spectral regions. Simultaneous analysis of the experimental and computational data show the dominant role of the Bi^{3+} and MoO_4^{2-} -related centers in intrinsic PL processes of studied compounds. The values of dielectric band-gaps E_g of the crystals are estimated from experimental data on diffuse reflectance spectroscopy. Formation of intrinsic PL excitation spectra and role of uncontrolled defects in PL processes are discussed.

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SPECTRAL AND SPATIO-TEMPORAL TRANSFORMATION OF ULTRASHORT LASER PULSES IN SELF-FOCUSING MEDIA

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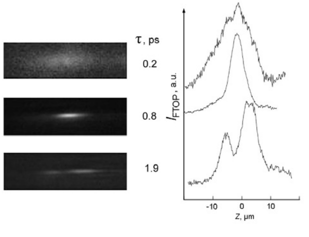
One of the most striking manifestations of spatio-temporal localization of light in transparent nonlinear optical media is filamentation. Extremely high power density (~ 10^{13} W/cm^2) at the filament axis promotes a large number of interconnected nonlinear processes, resulting in formation of the plasma channel, changes of the spectral composition and spatial and temporal distribution of the laser pulse. We report results of our study of the femtosecond filamentation in transparent Kerr media. Apart from transversal localization of the pulse, we also observe its temporal localization, followed by splitting into two separate successive pulses. We made a self-compression setup producing a temporally compressed probe pulse for pump-probe time-resolved measurements. Extraction of the compressed pulse component is carried out by diaphragm in a 200-fold expanded image of the filament "hot" core. 63 fs duration is achieved at the output, when the input pulse duration is 160 fs. We found parameters of the compressed pulse and optimized conditions for its excitation. Having used the compressed pulse as a probe for time-resolved measurements, we for the first time observed *in situ* in fused silica temporal self-compression of the femtosecond laser pulse in the filamentation mode, as well as its temporal splitting into sub- and superluminal subpulses. The figure shows instantaneous photos of the propagating pulse at different temporal delays τ and their corresponding longitudinal profiles. Observed spatial and temporal transformation of the propagating femtosecond pulse is qualitatively explained using the moving focus model and is consistent with the results of numerical modeling made by other authors.



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LUMINESCENCE OF CERAMICS ZnS-Mn

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Conducted in the last two decades of research within the center optical transitions in ions Mn, which are in different crystal matrices, lead to the conclusion that the properties of the electronic transitions depend strongly on the crystalline matrix, the concentrations of Mn, the excitation conditions and temperature. Intracenter radiation bivalent manganese is of practical interest because ZnS-Mn is the most effective electroluminescent phosphor. The study dose dependence of the luminescence ceramic ZnS-Mn is important for the creation of display devices, since they determine their radiation resistance.

The object of study was a fluorescent ceramics ZnS a concentration of 1% Mn in the blend. In the work, a study of the kinetics of photo-and X-ray luminescence with time (of dose) at steady-state irradiation of fluorescent ceramics ZnS-Mn. Excitation was carried out XRF X-ray tube radiation integral BHV-Re (20 kV, 25 mA), 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.

Small differences in half-width of the PL spectra of stationary radar and caused a no brainer main yellow band luminescence. It should be noted that the excitation power that was used in experimental studies, the intensity of photoluminescence stationary significantly exceed the intensity of X-ray laser. Zone-zone photo excitation crystals ZnS-Mn leads to highlight the light sum, as evidenced by significantly lower intensity of TSL in photo excitation compared with the intensity of the TSL under X-ray excitation. Dramatically uneven phosphor x-ray excitation leads to spatial heterogeneity of carrier localization at the centers, and most importantly, be dependent on the spatial coordinates as the future of the centers, and the ratio between the probabilities of recombination and re-localization of charge carriers. Of research shows that low-dose stimulation (2s.) phosphorescence decay is described hyperbolically with exponent $\alpha > 1$, and at higher doses (20min.) - hyperbole with $\alpha < 1$. It is obvious that such a feature of the dose dependences of the phosphorescence shows the local character of the luminescence excitation and accumulated light. 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.

PHOTO AND X-RAY LUMINESCENCE PROTON IRRADIATION OF CERAMICS ZnS-Cu

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The influence of stable radiating defects entered by a proton irradiation (doze of an irradiation 10^{15}p/sm^2 with energy 50 Mev) on luminescent properties of ceramics ZnS-Cu is investigated. In work used two sources of excitation: a photo - (LGI - 21, l=337nm) and integrated radiation x-ray tube (Mo, 35кV, 20 mA). Two sets of samples were selected: initial and irradiated by a doze 10^{15}p/sm^2 - described by fall of intensity stationary luminescence and strong reduction reserved of the light sum under curves phosphorescence and thermostimulated luminescence. The excitation was carried out at temperatures 85 and 295 K. The carried out researches of spectra of a stationary photo - and roentgen luminescence, testify to dependence of spectra luminescence from conditions of excitation in both sets of samples. The observable displacement of maxilla, and also difference in intensity of various strips of a luminescence, apparently, is connected that stimulating light is absorbed by the centers luminescence at - photoluminescence (impurity absorption), and basic substance at - roentgen luminescence. In the irradiated samples at X-ray excitation the intensity of a luminescence stationary roentgen luminescence has decreased on ~35 %, in particular of basic strip with a maximum l=522 nm. For photoluminescence of the irradiated samples the fall of intensity of a luminescence on ~10 % is characteristic. The main factors affecting the properties of semiconductor materials after irradiation with protons are the formation of new impurity as a result of nuclear reactions, radiating- defect production and accumulation of hydrogen atoms. The observable features of spectra of radiation at a photo and x-ray excitation can be caused by various spatial localization of energy of excitation on volume of a sample at presence of a various type is non-uniform of the distributed center of a luminescence, absorption and center's nonradiative recombination, and also various ways of transfer of energy of excitation by the center of a luminescence at various types of excitation because of redistribution of energy of excitation centre to centre luminescence of different grades. The redistribution recombination of flows of carriers centre to centre luminescence, absorption and centers nonradiative-recombination generated by a proton irradiation at X-ray excitation results in more significant fall of intensity roentgen luminescence in the irradiated samples.

RAMAN SPECTROSCOPIC STUDY OF $LiKB_4O_7$ SINGLE CRYSTALS

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The work is devoted to the study of Raman scattering spectra of new nonlinear optical $LiKB_4O_7$ crystals. The spectra were measured using a laser spectrometer based on double monochromator DFS-12 with registration in the photon counting mode and Renishaw inVia micro-Raman spectrometer. According to the results of the comparative analysis of the measured spectra with the spectra of $Li_2B_4O_7$, LiB_3O_5, β-BaB_2O_4 single crystals the assignment of vibrations in $LiKB_4O_7$ Raman spectra was performed. For some of the most intensive Raman bands, corresponding to the totally symmetric lattice vibrations, the estimation of the Raman scattering efficiency was performed. In the measured $LiKB_4O_7$ spectra there was observed a broad band of secondary radiation, which extends from the exciting line up to 5000 cm^{-1} and is probably caused by one of the nonlinear optical processes such as spontaneous parametric scattering of light.

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INFLUENCE OF CRYSTAL STRUCTURE IMPERFECTIONS ON THEIR PHYSICAL AND CHEMICAL PROPERTIES

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The aim of our studies was to investigate the effect of pulsed magnetic fields on the synthesis and properties of magnetite crystals.

In our studies, the synthesis was carried out by conventional magnetite precipitation method of crystallization from aqueous solution, containing ferric ions Fe^{+3} and Fe^{+2} in 1:2 proportion [1]. During the synthesis the dispersion medium was exposed to pulsed magnetic field (PMP), which was generated by electrical impulses, passing through the induction coil.

Investigations have showed that the magnetite crystals according to their structure belong to ferrous spinel [2]. The resulting precipitate has distinct crystalline structure. X-ray diffraction patterns of samples, exposed to PMP shows magnetite reflexes significantly broadened, which is so because crystals generation with less perfect structure and smaller size, comparing to control samples.

IR - spectroscopy showed that under the influence of PMP magnetite are synthesized with increased OH groups' quantity on the surface, as evidenced by broad absorption band near 3400 cm^{-1}, referred to valence oscillation of bonded OH groups. On the surface of natural and control group magnetites OH groups are allmost absent. Analyzing the data in [3] and comparing them with those obtained by us, we can conclude that the absorption bands near 590 and 440 cm^{-1}, associated with the lattice oscillations of Fe-O bonds in tetrahedral and octahedral of magnetite crystals, can be attributed to the oscillations of Fe^{+2} and Fe^{+3} ions. Weak absorption bands at 465 and 895 - 900 cm^{-1} can be attributed to the presence of magnetite Fe^{+3} ions as hydroxides, which are deposited on the magnetite surface.

Thus, during magnetite synthesis from aqueous solution, containing Fe^{+2} and Fe^{+3} ions, in alkaline medium under influence of pulsed magnetic fields it is obtained nanoparticles of magnetite crystals containing OH groups.

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STRUCTURAL, VIBRATIONAL AND THEORETICAL STUDIES OF ANILINIUM TRICHLOROACETATE: NEW HYDROGEN BONDED MOLECULAR CRYSTAL WITH NONLINEAR OPTICAL PROPERTIES

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In this work, we report a combined experimental and theoretical study on molecular structure, vibrational spectra and NBO analysis of the potential nonlinear optical (NLO) material anilinium trichloroacetate. The FT-IR and FT-Raman spectra of the compound have been recorded together between 4000-80 cm^{-1} and 3600-80 cm^{-1} regions, respectively. The compound crystallizes in the non centrosymmetric space group of monoclinic system. The optimized molecular structure, vibrational wavenumbers, IR intensities and Raman activities have been calculated by using density functional method (B3LYP) with 6-311++G(d,p) as higher basis set. The obtained vibrational wavenumbers and optimized geometric parameters were seen to be in good agreement with the experimental data. DSC measurements on powder samples do not indicate clearly on the occurrence of phase transitions in the temperature 113-293 K. The Kurtz and Perry powder reflection technique appeared to be very effective in studies of second-order nonlinear optical properties of the molecule. The non-linear optical properties are also addressed theoretically. The predicted NLO properties of the title compound are much greater than ones of urea. In addition, DFT calculations of the title compound, molecular electrostatic potential, frontier orbitals and thermodynamic properties were also performed at 6-311++G(d,p) level of theory. For title crystal the SHG efficiency was estimated by Kurtz-Perry method to be $d_{eff} = 0.70 d_{eff}$(KDP).

LUMINESCENT SPECTROSCOPY OF $Me_3LaNb_3O_{12}$ (M = Ba, Sr) LAYERED PEROVSKITES

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Spectral investigation of luminescence properties of the $Me_3LaNb_3O_{12}$ layered perovskites were carried out. The compounds have been obtained by heat treatment of co-precipitated hydroxy-carbonates. Co-precipitation was carried out in aqueous buffer solution with pH ≈ 8.5. In order to obtain single phase, shock heating thermal treatment was applied. Obtained structure was described using refinement of the model in the R-3 space group those gives satisfied values of the reliability factor (0,046). Crystal structure is formed by two-dimensional perovskite-like blocks each of them consists of three layers of the distorted MO_6 octahedrons, which are connected by vertices only. Luminescence spectra of these materials consist of wide bands in 350 – 650 nm spectral range. The peak positions of the spectra depend on the samples temperature and excitation wave length. It was found that luminescence emission is complex and contains strongly overlapped components at 430 and 500 nm. Intensity of these bands falls down with different rates with increase of temperature. We suppose that two observed luminescence bands are connected with two different types of niobate octahedrons, namely, inner-block (s) and corner-sharing octahedral niobate groups, respectively.

Luminescence properties were investigated using excitation with synchrotron radiation at SUPERLUMI station at HASYLAB, DESY, Hamburg, (Project # I-20110592) and complex for spectral-luminescent investigations at R&D Laboratory “Spectroscopy of Condensed State of Matter” at Physics Faculty, of Taras Shevchenko National University of Kyiv was used also. The investigations were supported by DFFD of Ukraine (Project # F54/040).

LUMINESCENCE STUDY OF MATRIX-ASSISTED ENERGY TRANSFER TO MATRIX-ISOLATED N_2 AND CO IN RARE-GAS SOLIDS

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The method of matrix isolation of reagents in inert matrix is usually used to study of chemical reaction molecular dynamics along with methods of molecular beams and femtosecond probing spectroscopy [1]. Matrix-assisted energy transfer to matrix-isolated species is one of the most powerful tools for photostimulated chemical reaction control, and rare-gas solids are the most popular media for such investigations [2]. In rare-gas solids the energy loss rate of photoelectrons with energies above the band gap energy is mainly determined by electron-electron scattering [3]. The scattering of a hot photoelectron by a valence electron results in the formation of an additional electron-hole pair which can be bound or free. Such processes of multiplication of excitations with well-defined thresholds lead to prominent structures in the photoluminescence excitation spectra. Rare-gas solids doped with N_2 and CO were extensively used to investigate intra- and intermolecular energy relaxation into the impurity subsystem. This paper reports the results of luminescence study of matrix-assisted energy transfer to matrix-isolated diatomic homo- (N_2) and heteroatomic (CO) impurity molecules in krypton and argon atomic cryocrystals.

The photoluminescence experiments were carried out at the SUPERLUMI experimental station at HASYLAB, DESY, Hamburg [4]. Rare-gas solids exhibit strong effects of neutral and charged defect formation induced by electronic transitions [2]. Therefore all measurements were carried out after saturation of dose effects at steady concentration of point defects and ionic centers. Under selective excitation by synchrotron radiation the threshold energies for multiplication of electronic excitations were measured. The energy ranges of impurity molecules photoexcitation were determined in which the channel of matrix-assisted electronic excitations energy transfer to matrix-isolated centers was most efficient.

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INVESTIGATION OF JAHN-TELLER PHASE TRANSITION IN KDy(MoO$_4$)$_2$ SINGLE CRYSTAL BY RAMAN SCATTERING

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Spectrum of the Raman light scattering is investigated in KDy(MoO$_4$)$_2$ single crystal in the frequency range 3–1000 cm^{-1} in the temperature range 2–300 K. Low-energy electron transitions between the levels of the crystal field splitted ground multiplet $^6H_{15/2}$ of the ion Dy^{3+} have been revealed. It is found that in the region of the first exited Kramers doublet of the ion Dy^{3+} (~ 22 cm^{-1}) a single line is observed in the high-temperature phase which is splitted below the phase transition temperature (14.5 K). At low temperatures the Raman spectrum in this region has a complex structure containing four lines.

At the transition to a low-temperature phase some additional phonon line appear in polarizations for A_g, B_{1g}, B_{2g}, B_{3g} modes, suggesting the doubling of the primitive unit cell volume under this transition. Examination of the polarization rules four the fundamental spectrum and the spectrum of additional lines suggests that below the phase transition the orthorhombic symmetry remains unchanged. It is found that the additional phonon lines appear at $T \sim 16.5$ K in contrast to $T \sim 14.5$ K at which the electron level begins to split and the Jahn-Teller phase transition occurs. Such a behavior of the scattering spectra suggests that there exist two successive phase transitions at different temperatures.

THE ISOCHORIC THERMAL CONDUCTIVITY OF CYCLIC MOLECULAR HYDROCARBONS

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Investigation of thermal conductivity is one of the tools of deriving information about the heat transfer mechanisms and general kinetic regularities in solids. In this context, of special interest are molecular solids possessing both translational and orientational disorders. Among diverse chemical molecular compounds having such properties, cyclic hydrocarbon systems are the most suitable objects because they can form different stable and long-lived metastable solid phases.

The thermal conductivity of cyclic hydrocarbons has been investigated in a series of experiments in a wide interval of temperatures (80K to melting) and pressures (20-140 MPa). The objects were:

- cyclohexene C_6H_{10} which can be obtained in orientationally – ordered and disordered phases and in a metastable phase
- furan C_4H_4O having two phases: orthorhombic orientationally-disordered phase I and tetragonal orientationally-ordered phase II. The purity of the substances (SIGMA-ALDRICH) was 99.0 % and 99.8 %, respectively. The dominant total systematic measurement error was up to 4 % for thermal conductivity and 0.2 % for volume.

It has been found that the isochoric thermal conductivity of cyclohexene in orientationally-disordered phase I increases smoothly with rising temperature. This behavior is typical of the «plastic» phases of molecular crystals and may be attributed to the phonon-rotation scattering component which reduces as the translation-orientation interaction grows weaker when the rotation of the molecules at the lattice sites enhances.

It is shown that the phonon component of the three phase states can be described adequately within the Debye-Peierls model taking into account the U-processes, phonon scattering at dislocations and point defects. Proceeding from experimental evidence it has been shown that the thermal conductivity of furan measured under the evaporated vapor pressure decreases as the temperature rises, this dependence being no stronger than 1/T. The isochoric thermal conductivity exhibits a weaker temperature dependence. The contributions of low-frequency phonons and «diffusive» modes to heat transfer have been calculated [1].

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PHOTOINDUCED CHANGES IN STRUCTURAL PROPERTIES OF PROUSTITE Ag_3AsS_3 UNDER LASER IRRADIATION

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Proustite Ag_3AsS_3 crystals are promising materials for nonlinear optics, so its investigation is well-developed in a wide temperature range – from helium to 600 K. It is important, that the effect of optical irradiation on physical properties of Ag_3AsS_3 is rather contradictory. That is why, in this work the temperature dependences of the unit cell parameters *a(T)* and *c(T)* of Ag_3AsS_3 were measured by X-ray dilatometry method with high precision in temperature range 100–300 K in dark mode and during laser irradiation (λ=532 nm). It was found that the parameter *c* increases almost linear with decreasing of temperature from 300 K to 100 K for samples it the dark. At the same time, for samples that were exposed during the cooling at the laser irradiation the increasing of the parameter *c* on the value of $\Delta c \approx (0{,}002–0{,}003)$ Å is observed at temperatures T_p=(145–147) K (Fig.1). This leap is typical for systems in which occurs a phase transition of the first order.

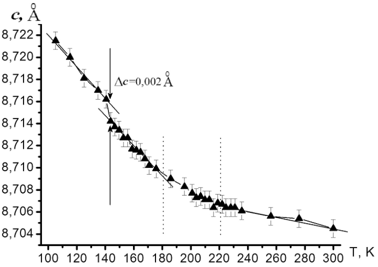

Fig. 1. The dependence *c(T)* under laser irradiation

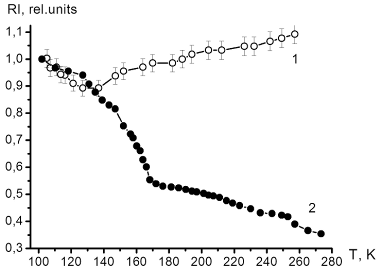

Fig. 2. The dependence *RI(T)* of maximum (312): 1 - dark mode, 2 - under laser irradiation λ=532 nm

Furthermore, there were investigated temperature dependences of the integral relative intensity (*RI*) of main structural maxima of Ag_3AsS_3 both in the dark mode and under laser irradiation. Earlier, we reported about anomalies on temperature dependences *RI(T)* of maxima (232), (202), (312) and (122) – the *RI* decreased while cooling samples from room temperature to T=150–160 K [1]. It was established the character of the dependence *RI(T)* for these reflexes changed significantly at laser irradiation. Namely, values of *RI* increase during the cooling from 300 K to 100 K. This effect is illustrated for maximum (312) on Fig. 2.

Thus, it was experimentally obtained the sensitivity of the unit cell parameter *c* to laser irradiation, shown the effect of optical irradiation on the temperature dependence of *RI(T).* Observed effects are explained in terms of the redistribution of silver ions on the two groups of vacant crystallographic positions in the unit cell.

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INFLUENCE OF POLYTYPISM ON STRUCTURAL PROPERTIES OF $TlGaSe_2$ CRYSTALS

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The ferroelectrics-semiconductor $TlGaSe_2$ are characterized by the pronounced layered structure and under normal conditions belong to the monoclinic system (the space group C^6_{2h}). Polytypic modifications of $TlGaSe_2$ crystals can be formed through the shift of one layer relative to the nearest layer by a distance equal to the edge of the $GaSe_4$ tetrahedrons along the edge of the large tetrahedron. This result in the formation of polytypes that differ in the number of layer stacks, i.e., in the *c* parameter: C, 2C, 3C, 4C…

It has been reported in many papers that for this crystals their structural peculiarities differs significantly for samples from various ingots. In particular, it concerns characters and temperature positions of ferroelectric phase transitions (PT). Such features were connected with the possible influencing of polytypism. In this connection the comparative X-rays researches of monocrystalline $TlGaSe_2$ samples which belonged to different polytypes (C and 2C) were performed in the temperature range T=100–300 K. Much attention was devoted to changes with the temperature of angular position, shape and number of (*00l*)-type reflections. By the X-rays dilatometry method it was shown, that for C-$TlGaSe_2$ polytype temperature dependence of the unit cell parameter *c*(T) is linear in the interval T=140-300 K and does not reveal hysteresis. The form of (*00l*)-type reflections does not change with temperature for this polytype. These results confirm absence of PT for C-$TlGaSe_2$ polytype at the mentioned temperatures range. At the same time for 2C-$TlGaSe_2$ polytype at the temperatures T<210 K dependence *c*(T) is nonlinear and the angle of dependence slope is increased with temperature decreasing. The changes of the (00.28) reflex shape of such polytype for the temperatures range below 240 K were revealed. The computer analysis of the indicated form reflex changes with the temperature allows supposing that the reason of form distortions is presence of modulation satellites. Angular position of such reflexes confirms existence of incommensurate modulated structure in crystals of 2C-$TlGaSe_2$ polytype below temperature 240 K. If take into account the features of ferroelectric PT in the two different polytypes of $TlGaSe_2$ crystals, reported by us earlier [1], the our experimental results prove the crystals of C-$TlGaSe_2$ are the ferroelectrics with an incommensurate phase of type I, and the crystals of 2C-$TlGaSe_2$ are characterized by incommensurate phase of type II.

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LUMINESCENCE SPECTRUM OF 2-(2’-HYDROXYPHENYL) BENZOXAZOLE IN THE SOLID STATE

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2-(2’-hydroxyphenyl)benzoxazole (HBO) undergoes excited state proton transfer (ESIPT) upon photoexcitation. In the ground state HBO can exist in two rotameric forms with intramolecular hydrogen bonds (OH...N and OH...O), only the structure with the OH...N hydrogen bond undergoes ESIPT and demonstrates fluorescence with a large Stokes shift (keto fluorescence) [1]. Conformational disorder (approximately equal numbers of the OH...N and OH...O structures) has been reported for the crystal of HBO basing on X-ray measurements [2] but the study of the IR spectrum of solid state HBO in the region of intramolecular vibrations has not found the bands which could be assigned to vibrations of the OH...O rotamer [3].

We have studied a luminescence spectrum of polycrystalline HBO in the region of the normal and large Stokes shift. The luminescence spectrum of HBO dissolved in CCl_4 at room temperature demonstrates an intense band with a maximum at 504 nm and a weak band at 357 nm. In the spectrum of polycrystalline HBO only a band at 504 nm is observed, its position and shape are similar to one in solution. Quantum chemical DFT calculations performed for various rotameric and tautomeric structures of the isolated molecules of HBO predict that the equilibrium number of the OH...O species in the ground state is of the order of 10^{-5} in relation to the number of the OH...N species. TDDFT calculations of the excited states of the isolated molecules show that the emission of the OH...O rotamer can be quenched by energy transfer in the crystal, whereas the keto fluorescence is enhanced by restriction of large-amplitude twisting of the molecule [4].

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PECULIARITIES OF THE CRYSTAL GROWTH OF THE 2-ACETYLDIMEDONE BORIC CHELATE MEROCYANINE DYES UNDER DIFFERENT CONDITIONS

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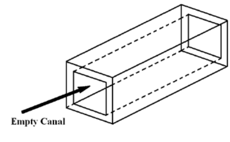
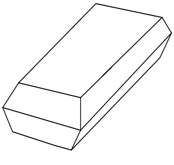
In the view of the possibility of practical application of the merocyanine dyes and their analogues unrelenting interest in them develops. These dyes serve as NLO-materials and could be used in OLED displays production. For the investigation of the correlation structure and spectral-fluorescent properties of merocyanine dyes, 2,2-difluoro-1,3,2(2H)-dioxaborine dye was synthesized.

It was found, that these dyes depending on conditions could be crystallized in two forms: classic single crystals and crystals with through canals inside. In the most cases these canals reiterate the outward form of crystals and their size varies depending on the solvent compound was crystallized from. The crystallization from the alcohols under normal conditions leads to the formation of “tubes” (the hollow size ca. 0.06x0.06 to 0.15x0.15 mm in section). The using of solvents such as acetonitrile causes the growth of classic single crystals (prism form). With the imposition of the external electromagnetic field up to 750 kV/m on the specially designed device «Kristall-W 4.0» all crystals have a classic form undependent on any solvent type, but they become thinner and notably longer than without the field (coffin form).

It is worth to note that the indexing of X-ray reflections for the both types of crystals (with canals and single crystals of classic form) give the same cell parameters. It means that structure of crystals with canals isn’t generated in the way of growing of different facets together. It is possible that crystals’ growing was caused by the specific influence of proton-donor solvents which able to block separate parts of molecules of dye in such a way that crystals growth on the free of salvation areas of compound occurs. The application of the external electromagnetic field changes the surface energy of the germ, so crystal shape changes to the coffin form.



Scheme of the crystal with canal



Scheme of the coffin form crystal

MOLECULAR AND CRYSTAL STRUCTURE OF 3-TRICHLOROMETHYL-4,5-DIHYDRO-1,2,4-BENZOTHIADIAZEPINE-1,1-DIOXIDES

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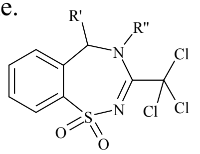
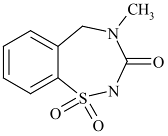
In contrast to well studied relatives 5-membered 1,2,4-thiadiazoles and 6-membered 1,2,4-benzothiadiazines heterocycles peculiarities of structure 7-membered heterocycles are still on the question. In this work we report results of single crystal X-ray investigation of recently synthesized [1] compounds **1-5** with 7-membered cycle which are perspective as new therapeutic agents in medicine.



1: R' = H, R" = CH_3 ; **2**: R' = H, R" = $(CH_3)_2CH$;
3: R' = H, R" = H; **4**: R' = CH_3 , R" = H.



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It was found that the conformation of 7-membered heterocycles SN_2C_4 strongly depends on the substituents properties. The structures **2, 3, 5** have conformation of *envelope* (the fragments SN_2C_2 and SC_3 are planar with the dihedral angle 59.9° (**2**), 57.2° (**3**), 39.76°(**5**)). In contrast to **2, 3, 5** the particularity of the structure **1** is strongly distorted *twist*-conformation (the torsion angles varies in the range 7.9 ° -80.4 °) whereas the heterocycle SN_2C_4 of **4** is planar within 0.06 Å (Fig.1).

Interesting feature of the crystal packing of **1** is intermolecular stacking (Fig.2), while the molecules **2**, **3**, **5** are organized in dimmers by π-π interaction (Fig.3) (some substituents are omitted for clarity).

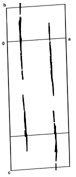

Fig.1

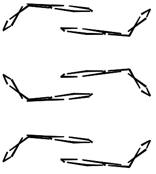

Fig.2

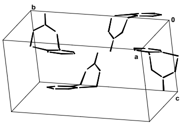

Fig.3

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OPTICAL CONSTANTS OF CdZnTe FILMS ON SILICON

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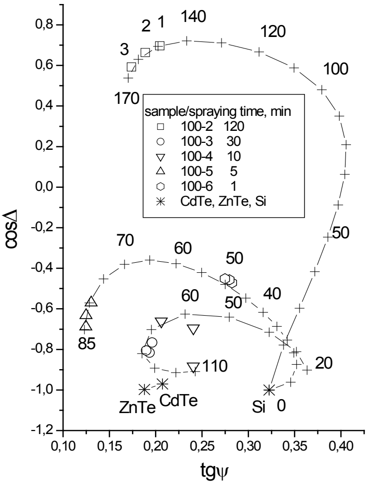
It was the purpose of the given work to explore, as change ZnCdTe films optical constants and their heterogeneity with the increase of time of spraying. Films CdZnTe are got on the monocrystaline silicon by the “hot wall” method. Composition of charge made: 44,8Cd, 53,729Te and 1,468Zn atomic percents. Films are inflicted during 1, 5, 10, 30 and 120 minutes. Films have a different interference color, that is a different thickness, on an area. Data of atomic power microscope testify that films are granular with the size of corns from 30 to 500 nm for the spraying times from 1 to 120 minutes.



On the wave-length 632,8 nm ellipsometric parameters is measured, the indexes of refraction and absorption and thickness are found. The results of measuring are given on figure by symbols. Curves are calculated after found optical constants. Numbers near the curve ticks indicate the films thickness in nanometers. Experimental points are laid on three separate curves that answer different optical constants. Samples with time of causing 1 and 5 minutes (with a thickness from 50 to 80 nm) have the index of refraction 2,7, index of absorption 0,67. With the increase of spraying time from 10 to 30 minutes the films with the index of refraction 2,94 and index of absorption 0,8 are formed. Finally for a sample with spraying time 120 minutes the index of refraction slumps to 1,75.

As CdTe absorption index – 0,4, increase of his value to 0,8 testifies that explored films contain the high-absorptive material, it is possible telour, in the free state.

OPTICAL PROPERTIES OF PARA-BROMBENZOPHENONE POLYMORPHS

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In a comparative study of optical properties of the two known polymorphs (monoclinic and triclinic) of para-bromobenzophenone, including integrated and time-resolved phosphorescence spectra as well as singlet-singlet and singlet-triplet absorption spectra have been measured at three temperatures 293, 77, and 1.6 K. The relevant kinetic parameters have been determined. At room temperature (293 K) the in both forms have a clearly monomeric character with close values of the energies that correspond to the maxima of the C=O vibration bands. The 0-0 band emission relaxation times differ substantially. The integrated spectra at 77 K are also of monomeric character and have close 0-0 band relaxation times.

The general view of the integrated phosphorescence spectra of both polymorphs at 1.6 K is also monomeric. However, the low-energy part of the 0-0 bands in both polymorphs shows narrow spikes ascribed to exciton emission from some traps as well as narrow low-intensity bands of free excitons. Proceeding from the actual structure of the two polymorphs [1], a one-dimension model is suggested [2] within which the corresponding tunnel spectra of triplet excitons have been calculated using the tight-binding approximation. This enabled us to conclude that the triplet exciton band width Δ in the T-form is approximately 4 times larger than in the M-form. Hence, the tunneling diffusion coefficient, which is proportional to Δ^2, in the T-form should exceed by an order of magnitude the corresponding value in the M-form. Comparative analysis of the integrated spectra gives grounds for the conclusion that diffusion in the T-form is essentially more efficient, in correspondence with qualitative inferences of our theory.

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HEAT TRANSFER IN “PLASTIC” PHASES OF CYCLIC HYDROCARBONS

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Here we present the study of the isochoric thermal conductivity in “plastic” phases of solid furan (C_4H_4O) and cyclopentane (C_5H_{10}). The thermal conductivity has been measured at isochoric conditions for samples of different densities. It increases with temperature in furan and cyclopentane (I) and is nearly constant in C_5H_{10} (II). Such behavior is attributed to weakening of the translational orientational coupling which, in turn, leads to a decrease of phonon scattering on rotational excitations.

Furan molecule is a planar five-membered heterocycle with one oxygen atom. It has a phase transition at 150 K with an entropy of transition $\Delta S_{I-II}/R=1.6$ and melts at 187.6 K with entropy of fusion $\Delta S_f/R=2.3$ indicating that the high temperature phase of C_4H_4O can be attributed to a “plastic” crystal [1].

Cyclopentane (C_5H_{10}) is a cycloaliphatic organic molecule consisting of the ring of five carbon atoms with two hydrogen atoms above and below the plane of carbon skeleton . Molecule can exist in two essentially isoenergetic puckered-ring conformations: half-chair, C_2 and bent, C_S that are in dynamic equilibrium and interconvert by an isoenergetic process called pseudorotation [2]. Cyclopentane has two phase transitions at 122.4 K and at 138.1 K with entropy of transitions $\Delta S_{II\rightarrow III}/R=4.8$ and $\Delta S_{I\rightarrow II}/R=0.3$ respectively, and melts at 179.7 K with entropy of fusion $\Delta S_f/R=0.4$ implies that phases I and II of cyclopentane are “plastic” crystals and that they are only slightly more ordered than the liquid state [3].

The structure of solid furan and cyclopentane was studied using X-ray single-crystal, X-ray powder and neutron powder diffraction [4]

Crystallographic structure of furan was determined by R. Fourme, M.J. Wyart [5]. In phase I each molecule occupies randomly four coplanar positions. Dielectric [6] and nuclear magnetic resonance [3] studies have shown that disorder is dynamic and that molecules reorient rapidly between four allowed orientations. In phase II the structure is ordered in the sense that each molecule has only one allowed orientation. Earlier the thermal conductivity of furan was studied at constant pressure 0.11 and 1.2 GPa [1].

Phase I of cyclopentane has a hexagonal space group with two molecules per unit cell. Phase III has a monoclinic unit cell P_1/c with Z'=1. The neutron powder pattern from phase II showed a significant background contribution indicative of a disordered plastic crystal with a large unit cell, or maybe incommensurate, however, the exact structure has not been determined.

Isochoric measurements were carried out on a device with coaxial geometry using a stationary method. Purity of studied samples was no worse than 99,8%. The measurement error was ±4%.

Was found that in phase II the isochoric thermal conductivity of hydrocarbons is practically temperature – independent, but it grows smoothly with temperature with temperature in phase I. We attribute the growth of thermal conductivity with increasing temperature to the translation – orientation interaction which becomes weaker as the rotational motion of the molecules enhances and the phonon scattering at the rotational exaltations attenuates. Thus, we can conclude that disinhibition of uniaxial rotation of the molecules in the cyclic hydrocarbons leads to the increase of the thermal conductivity with temperature like "plastic" phases of other molecular crystals [7].

The increase of thermal conductivity with temperature can be attributed to a weakening of the translation orientation coupling when the rotational motion of molecules.

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BIREFRINGENCE OF UNIAX CRYSTALS FROM CARPATHIAN MOUNTAINS

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Uniax plates of solid crystalline substances are characterized by two principal refractive (ordinary and extraordinary) indices. When polarized light passes through uniax plate perpendicularly on the optical axis, its birefringence can be determined by compensation of the pathway introduced between the ordinary and extraordinary components of the incident linearly polarized light. In order to estimate the birefringence of the samples collected from Carpathian Mountains, we used both a Babinet Compensatory and a standardized optical wedge in order to compensate the pathway at 589.3 nm introduced by layers cut perpendicular on their optical axis. The results were compared with those obtained by using the method of channeled spectra.

The dispersive properties of Carpathian Quartz regarding the main refractive indices and the rotatory power were established on the basis of the measurements in the channeled spectra obtained with visible radiations. The curve describing the dispersion of the main refractive indices and of the birefringence is of the Cauchy type, but the dispersion of the rotatory power varies linearly with the wavelengths in the small spectral ranges, having variable slopes of variation.

DYNAMIC AND STATIONARY PROPERTIES OF PHOTOINDUCED LIGHT SCATTERING IN LiNbO$_3$: Fe CRYCTAL WITH SUPERCONTINUUM EXPOSURE

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Analysis of photoinduced light scattering (PILS) in photorefractive (PR) crystal allows one to get detailed information about the mechanisms of photorefractive gratings formation / 1, 2 /. PILS research under supercontinuum radiation in PR crystal LiNbO$_3$: Fe conduct for the first time. This crystal has a unique photovoltaic property in the visible and near infrared optical bands. Supercontinuum (SC) is a coherent broadband radiation. Spectral broadening occurred by passaging of femtosecond pulses in a highly nonlinear microstructured (MS) fiber. Stable generation of SC in the spectral range 530-1000 nm with an average output power 200 mW was obtained in MS fibers with pumping pulses from femtosecond Ti:S laser Mira Optima 900-F / 3 /.

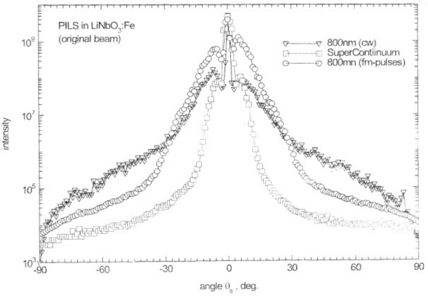

Figure. 1. Light scattering angular dependence of LiNbO$_3$: Fe crystal.

As part of the comparison of the angular dependence of light scattering (see Fig. 1), gain coefficients and scattering dynamics exposing LiNbO$_3$:Fe crystal with monochromatic light sources (Ti:S laser in femtosecond and continuous operation mode) and polychromatic SC radiation we determine the effectiveness of the PR response in different spectral ranges.

Maximum PILS intensity observed:

- At 6° angle for femtosecond SC (550 - 900 nm),
- At 8° angle for femtosecond Ti: S laser (800 nm) for continuous and pulsed operational regimes.

Qualitative difference in PILS induced by SC pronounced in light angular scattering selectivity. Photorefractive parameters value obtained for SC in order of magnitude coincide with those for the monochromatic sources. In conclusion, we makes assumption about possibility for holographic multicolored holograms recording in $LiNbO_3$:Fe crystal with SC radiation and evaluate possible advantages and disadvantages compared with conventional monochromatic schemes.

This work was supported by grant RFFD/NASU, № 42-02-12 (U).

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5
LIQUID CRYSTALS

SELECTIVE REFLECTION IN CHOLESTERYL OLEYL CARBONATE(COC)-NEMATIC 5CB MIXTURES AND EFFECTS OF THEIR DOPING BY SINGLE-WALLED CARBON NANOTUBES

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Liquid crystalline (LC) mixtures of cholesteryl oleyl carbonate (COC) and 4-pentyl-4’-cyanobiphenyl (5CB), as well as dispersions of single-walled carbon nanotubes (NTs) in these mixtures, were studied by means of selective reflection measurements, differential scanning calorimetry (DSC) and optical microscopy. The relative mass of COC in a mixture X was varied between 0.4 and 1.0, the temperature range of measurements was between 284 K and 314 K, and concentration of NTs was fixed at 0.1 %. Two important anomalies were noted: (1) the cholesteric to smectic-A transition temperature increased on dilution of COC by non-smectogenic 5CB in the concentration range $0.8<X<1$, and (2) the reciprocal pitch vs. 5CB concentration dependence was essentially linear, in contrast to behaviour commonly observed in nematic-cholesteric mixtures. A model of molecular arrangement in the mixtures, accounting for the possibility of integration of 5CB dimers and monomers between COC molecules and presumably explaining the experimental data, was proposed. The helical pitch of the cholesteric mixtures remained practically unchanged upon doping by NTs, and only slight widening of the selective reflection peaks was noted. The obtained results allow considering the COC+5CB mixtures as promising matrices for composite materials on the basis of liquid crystals and carbon nanotubes.

OPTICAL TRANSMISSION AND DIELECTRIC PERMITTIVITY IN NEMATIC LC DISPERSIONS OF CARBON NANOTUBES (CNT): EFFECTS OF CNT TYPE AND CONCENTRATION

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Optical transmission as function of temperature, as well as dielectric permittivity in the 50 Hz – 1 MHz range, were studied for dispersions of carbon nanotubes (CNT) in nematic 5CB. Several types of CNT (multi-walled - MWCNT, single-walled - SWCNT, as well as double-walled and chemically modified CNT) were used, with their concentration varying from 0.01% to 0.5% in LC cells of 10-50 micron thickness. The measurements were carried out just after ultrasonication (a UZD 22/44 disperser) and after several hours to assess the time stability of such systems as potential functional materials.

In a broad range of parameters, the optical transmission of the dispersions studied in the nematic and isotropic states generally followed the Bouguer-Lambert-Beer law, with certain noted deviations indicating the onsets of structural transformations in the system (aggregation, sedimentation, etc.). Clear differences in the effective extinction coefficients could be noted for MWCNT and SWCNT, explicable from the viewpoint of the assumed supramolecular ordering.

The most striking were the effects of MWCNT and SWCNT upon dielectric permittivity, with marked differences at lower and higher frequencies. At frequencies below ~10 kHz, the dispersed CNTs acted as charge carrier traps, with noticeably larger specific area of SWCNTs at the same concentrations. These results can be considered as a natural extension of those obtained in [1], when nematic LC with high and low content of ionic impurities were compared in a similar way.

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POLARIZATION-SENSITIVE GRATINGS IN A LIQUID CRYSTAL CELL WITH CHALCOGENIDE ALIGNING SURFACE

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We present polarization gratings that are recorded in a combined 30 μm liquid crystal (LC) cell with a photosensitive chalcogenide film as a command layer. The reference substrate is covered with a rubbed polyimide film. The gratings are recorded with two beams of opposite circular-polarizations due to formation of spatially-modulated easy orientation axis, ***e*****,** on the command surface. The axis ***e*** on the chalcogenide surface is characterized by a weak anchoring and the reference surface provides a strong anchoring with the LC.

Several diffraction orders of the equal intensity in the each order are observed. The polarization of the ±1 order diffraction beams are elliptically polarized with the long axis at the angle *π/4* to the rubbing direction, and the polarization of the zero order is of the same ellipticity but oriented at the angle *–π/4* to the rubbing direction. The sign of the polarization rotation of the zero order and the diffraction orders coincided with the sign of the rotation of the probe.

Erasure of the diffraction grating by one of the recording beams after a switching the other beam off and a following re-recording are observed. The diffraction efficiency of the grating is of the order of few percents and is controlled by application of *ac* electric field. The highest efficiency of the first orders diffraction, $\eta \approx 90\%$, is achieved at the voltage 10V.

Analyses of the diffraction of a circularly polarized probe, that propagates from the side of the reference substrate, shows the unique properties of the gratings, the diffraction intensity is spectrally insensitive, does not depend on optical properties of the LC, and it is only determined by the anchoring of the LC with the surface. The necessary condition for formation of such grating is a weak anchoring of the LC on the command surface.

SPECTRAL AND THERMOTROPIC PROPERTIES OF H-BONDED LIQUID CRYSTALS INCORPORATED INTO MESOPOROUS INORGANIC MATRICES

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Among the brightest representatives of nanostructured composite materials are porous matrix filled with liquid crystal (LC). The unique physical properties of such LC nanocomposites originate both from the influence of the confined geometry, and the nature and concentration of the active sites on the inorganic porous matrix surface. Since the stability of composite 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 mesoporous inorganic matrices of different structure and morphology. The two types of porous matrices were used: porous silicate glass (PG) with controlled pore diameter (2 to 90 nm average pore size), and aluminosilicate molecular sieves MCM-41 with 4 nm pores. As H-bonded LCs were used *n*-alkylbenzoic (ABA) and *n*-alkyl cyclohexanecarbonic acids (ACHA) with *n*=2-6, where *n* is the number of carbon atoms in the alkyl radical, together with commercial LC mixtures CC-3 and PC-29 comprising various homologues of ABA and ACHA were used. By temperature-variable FTIR spectroscopy (Bruker IFS-88, 2 cm-1 resolution, 20-200ºC) and differential scanning calorimetry (DSC, Perkin-Elmer DSC-7, -100-200ºC) the influence of pore size and physico-chemical state of the surface on the LC ordering in the porous matrices is investigated. It is shown that phase transition temperatures for the H-bonded LC confined to PGs are nearly the same as those in the bulk, while LC confined to MCM-41 show thermotropic behavior significantly different from that observed in a bulk material. For the first time, a spontaneous dissociation of the hydrogen-bonded LC near the MCM-41 surface due to interaction with the surface active sites.

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ELECTRO-OPTICAL RESPONSE OF A POLYMER DISPERSED FERROELECTRIC LIQUID CRYSTAL FILM

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Polymer dispersed liquid crystal (PDLC) films are interesting materials since they exhibit promising electro-optic properties such as wide viewing angle and high brightness which are ideal for flat panel display devices [1-3]. In their most common form, PDLC materials consist of micron-size droplets of a low-molecular weight nematic liquid crystal dispersed in a polymer matrix. These materials operate on the principle of electrically controlled light scattering. The optical properties of a polymer dispersed liquid crystal films can be controlled by the application of external electric fields. PDLC devices do not need polarizers and they are easy to manufacture. However, the response of a nematic liquid crystal to the applied electric field is slow and this is also one of the drawbacks for its potential use. Thus, efforts have also been made to use ferroelectric liquid crystals which are known for very fast switching properties for display applications [4]. Recently, polymer-dispersed ferroelectric liquid crystal (PDFLC) devices have been proposed and successfully produced [5-7]. In this work fast switching PDFLC films were prepared and their electro-optic properties were investigated. PDFLC materials were prepared by a polymerisation induced phase separation technique of mixtures composed of an ultraviolet cured polymer and a difluorterphenyl ferroelectric liquid crystal. The liquid crystal droplets were aligned by shearing during the phase separation. The electro-optical response of the PDFLC films was investigated. The PDFLC films showed a fast and bistable switching as a function of the applied electric field**.**

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FORMATION OF LIQUID-CRYSTALLINE PHASE IN SILICON-ORGANIC POLYMER

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We studied a change of PDHS films conformation and orientation as well as a formation of the defect states arising during the annealing of the poly(di-n-hexylsilane)- PDHS at temperature close to the transition to the liquid-crystalline (LC) phase. It was investigated the appearance of the LC phase and its transformation depending on the thermal treatment temperature (20-180° C) and polymer molecular weight (M_w) using the absorption spectra, a polarising optical microscope and thermostimulated luminescence (TSL) in the temperature range 5-250 K.

It was shown that the formation of the LC phase upon continuous heating of the film from room temperature up to 180°C is associated with the appearance and the transformation of the positions and intensities of two new absorption bands in the region of gauche conformation.

The presence of the LC phase is also confirmed by the visual observation of the optical texture observed in the 57-140° C temperature range. The texture corresponds to the classical columnar liquid crystal ordering. It should be noticed that the texture remains for a long time after the annealed film is cooled to room temperature.

In addition, in the spectrum of TSL of annealed PDHS film after cooling to the room temperature a new wide band arises. It shifts from the spectrum of neat polymer film towards higher temperature indicating an appearance of the deeper traps. This band is probably caused by the defect states related to residual phenomena arising after the transition of thermally treated polymer film from the LC state to trans-conformation.

It was shown that the formation of the LC phase essentially depends on the M_w of the polymer. This phase is good obtained on the film with M_w=53000, and not good for large and smaller M_w, probably due to preventing the processes of reorientation and ordering of the polymer chains.

DISPERSIONS OF CARBON NANOTUBES IN CHOLESTERIC LIQUID CRYSTALS: OPTICAL AND ELECTROPHYSICAL STUDIES

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Dispersions of carbon nanotubes (CNT) in cholesteric liquid crystals (CLC) were studied. The main purpose was determining time stability of such systems as potential functional materials. The main factor affecting time stability is formation of CNT aggregates after ultrasonication.

Three main parameters were checked as characteristics in monitoring of the aggregate formation: (1) jump in optical transmission at the temperature of transition to the isotropic phase, (2) decrease in electrical conductivity with time, (3) conductivity changes under dc voltage in the geometry of Freedericksz transition.

Dispersions of CNT in nematic 5CB were taken as reference samples. It was found that addition of chiral components to the nematic matrix led, in all cases, to changes in the time dependences of the measured parameters due to changes in the aggregate formation kinetics.

Thus, the characteristic optical jump at the isotropic transition, which became noticeably smaller after 6 hours for 0.1% CNT in 5CB, remained almost unchanged after 24 and 72 hours when 5% of a mixture of cholesterol esters was added to the initial 5CB. Relative electric conductivity of 5CB+0.1% CNT dispersion decreased by 2 times after 5 hours, while similar dispersions in 5CB doped with 5% R-811, 5% of mixture of cholesterol derivatives (80% cholesteryl oleyl carbonate + 20% cholesteryl chloride – COC/CC), 30% of COC/CC and pure COC/CC after 25 hours showed decreases by 40%, 20% and <5%, respectively. Also, introduction of 5% COC/CC noticeably stabilized in time the Freederickcz transition parameters.

The results obtained are discussed in terms of interaction features between CNT and mesogenic molecules. It is argued that cholesterol esters, especially long-chained COC, can be considered as analogs of ‘tailored compounds” used in [1,2] for stabilization of nematic CNT dispersions.

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LIGHT-SENSITIVE AZOPOLYMERS AS LC PHOTOALIGNMENT AGENTS

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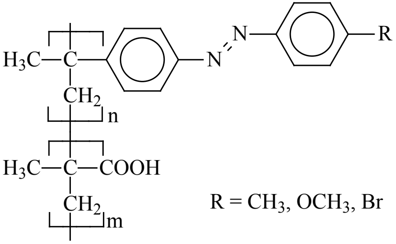
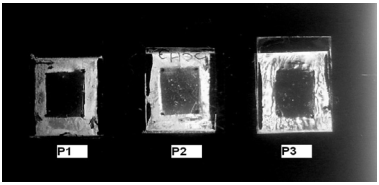
Among topics for polymer materials the development of light-controlled high-sensitivity polymeric systems is a very important problem nowadays. Control of optical properties of polymeric materials after their light exposure has significant advantages over electrical and magnetic fields action. In applications it is more convenient for the use in recording-reading machines, for easier polymer processing and thin polymer films preparation [1,2].

We obtain light-sensitive polymers based on polymethacrylic acid, containing azofragments and carboxylic functional side-chain groups. By methods of polymer-analogous transformations, particularly by condensation of its carboxylic groups with hydroxyazobenzenes, polymethacrylic acid, where part of the carboxylic functional groups were transformed into photochromic moieties, such polymers were synthesized.



R = CH_3, OCH_3, Br



All obtained polymer films are found can be orientated under polarized light and than orientate liquid crystals , covered with them, as it"s seen on photoes.

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NEW CHOLESTERIC LC MIXTURES FOR BISTABLE REFLECTIVE DISPLAYS

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Bistable cholesteric liquid crystal (LC) display technology has growth potential since such displays do not need a backlight, possess memory property and can be flexible [1, 2]. For these purely reflective displays of next generation the cholesteric material consisting of a nematic LC and a chiral dopant must have a complex of characteristics that makes it a sophisticated system.

In present work we discuss the results concerning cholesteric LC mixtures on the base of several commercial nematic LCs possessing low threshold voltages and including low concentration of new chiral dopants (5-7 wt. %) of steroid type. The influence of molecular structure of chiral dopants on helical twisting power in LC mixtures, photostability, solubility and dependence of desired reflective wavelength on temperature is investigated.

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NANOOBJECTS

NANOSCALE APATITE BIOMATERIALS FOR OSTEOINTEGRATION

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Nanoscale crystalline particles of biogenic apatite bone have a complex ultrastructural organization, which is caused by their functional purposes. Reconstruction of such structure in artificial materials for osteoplastics is impossible. These circumstances are stimulated the study of natural bone apatite as a source of biological material.

To prevent an immune response the organic component of donor bone tissue can be removed by pyrolysis, chemical treatment or a combination thereof. At the same time until the last minute the problem of optimization treatment procedures for maximum removal of organics with minimal changes of biomineral remains. Nanocrystalline bioapatite with preserved natural properties can be a base material for the development of artificial mineral organic composites for osteointegration with severe osteoconductive and osteoinductive properties.

This work was carried out to detailed study of the effect of heat treatment on the microstructure (the crystallite size and lattice microstrain), ultrastructure (habitus, orientation, impurities), and the natural bone architecture (osteon-lamellar structure). As a result, new technology for the production of nanostructured materials based on natural bioapatite has been developed.

Samples of bone tissue, obtained during development technology, were characterized using physical complementary approaches that were available by combining the following methods: X-ray diffraction, scanning electron microscopy with X-ray microanalysis, X-ray photoelectron spectroscopy and differential dissolution.

The need for development of this technology is caused by a significant number of patients with cancer and degenerative bone diseases, for which use artificial bone substitutes.

TIME-RESOLVED OPTICAL SPECTROSCOPY OF ATOMICALLY PRECISE CdSe NANOSTRUCTURES

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Significant progress in synthesis of CdSe nanostructures with the atomic precision, namely, magic clusters of exact number of constituting atoms [1] and nanoplatelets of definite number of atomic layers [2], allows fine details of optical properties of the nanostructures to be measured on an ensemble of them, while such studies were possible only for single particles yet.

The samples, aqueous colloidal solutions of magic clusters of $(CdSe)_{33,34}$ stabilized by cysteine, and powders of cadmium octanoate with enclosed nanoplatelets of 5 or 6 CdSe monolayers, have been prepared according to [3] and [4], respectively.

Photoluminescence measurements in 500fs – 500ns time domain and pump-probe absorption studies with subpicosecond resolution, performed at Femtosecond Laser Center for collective use of equipment of NAS of Ukraine [5], allowed us to investigate kinetics of excitons in 0D and 2D CdSe systems, and to observe manifestation of nonlinear optical phenomena in the systems.

Obtained results will be useful for deeper understanding of structure and properties of CdSe nanoobjects, thus opening new applications.

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RAMAN SPECTRA OF GRAPHENE-LIKE NANOPARTICLES OF TRANSITION METAL DISULFIDES

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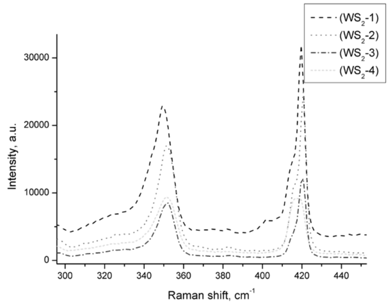
Two-dimensional (2D) nanomaterials have received much attention in recent years due to their unusual properties associated with their ultra-thin thickness and 2D morphology. Recent research on graphene has created interest in preparing and characterizing graphene analogues of layered inorganic materials for their applications in nanoelectronics, optoelectronics, energy storage etc

Here we report the successful results obtained in the case of $MoSe_2$ and WSe_2. Graphene-like nanoparticles were obtained with the use of laboratory nanotechno-logy using chemical vapor deposition (CVD). This technology allows to fabricate homogeneous graphene-like-2H-TMS_2 in sufficient quantities with extremely small average size of anisotropic nanoparticles (~1 nm to [013] crystallographic direction).

The spectra were detected by an automated double spectrometer DFS-24 (LOMO, Russia), equipped with a cooled photo multiplier and registration system working in a photon counting mode. Spectra were excited using Ar^+ laser with the wavelength of 514.5, 488 and 476.5 nm and power of ~50mW.



Raman spectra of graphene-like nanoparticles of 2H-WS_2 and 2H-MoS_2 as well as micron powder of natural 2H-MoS_2 for comparison have been investigated. We studied the intensities and shifts of Raman peaks as a function of the number of layers (2–8) and laser excitation.

Aknowledgements

We thank L.G.Akselrud from Ivan Franko National University of Lviv for X-Ray spectroscopy investigation of the samples.

DISTRIBUTED FEEDBACK LASER BASED ON DYE-DOPED VOLUME BRAGG GRATING HOLOGRAPHICALLY INDUCED IN PHOTOCURABLE NANOCOMPOSITE

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Recent development of new organic and composite materials and low-cost methods for fabrication of periodic micro- and nanostructures resulted in cost-efficient, maintenance-free tunable microlasers based on permanent distributed feedback which can be integrated onto optical and fluidic microchips usable for medical and biosensing.

Polymer DFB laser under study is a planar waveguide containing a volume grating doped with a laser dye. In this work we experimentally investigated the influence of the waveguide and grating parameters on spectral and energy characteristics of this kind of DFB laser in order to improve lasing parameters.

The gratings were formed by holographic structuring of the photopolymerizable nanocomposite containing the $LaPO_4$ nanoparticles (NP) and activated with a Pyromethene 567 laser dye. The grating periods were matched to second-order operation. The active gratings were pumped with a frequency-doubled Nd:YAG laser which emits 500 ps long pulses at a wavelength of 532 nm. Spectral and polarization properties, input–output characteristics of the laser were investigated by varying the material composition and the patterning parameters. By optimizing the material and the feedback structure, a narrow line-width oscillation with the threshold pump energy of 0.2 μJ/pulse was achieved for the second Bragg order lasing. The wide-band tuning of the DFB laser output from 568 to 625 nm has been demonstrated due to the variation of the grating period.

The lasing emission spreads from an active layer into the substrate and goes out from the substrate edge. The spatial intensity distribution in the output beam has an almost Gaussian profile and the beam divergence was found to be ~ 5 mrad. The emission out-coupling provides by second order Bragg diffraction of the waveguide mode by the grating.

This work was supported by the grant of the National Target Scientific and Engineering Program “Nanotechnologies and Nanomaterials” (Project 1.1.4.13/13).

PRO-OXIDANT AND ANTIRADICAL PROPERTIES OF RARE-EARTH BASED NANOPARTICLES EVALUATED BY CHEMILUMINOMETRY

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Recently, successful biomedical applications of RE-based nanoparticles (NPs) have been demonstrated. Bright luminescence, low toxicity and facilitated functionalization enable their use as imagine agents and nanocarriers. CeO_2 and other NPs are potent, and probably regenerative, free radical scavengers *in vitro* and *in vivo*. For example, CeO_2 NPs either can demonstrate UV and radiation-shielding properties [1, 2] or can induce oxidative stress [3]. Beside of reversible oxidoreduction processes RE ions can be exploited for oxidant detection [4].

Reaction activity of NPs depends on their size, shape, chemistry, synthetic procedure, etc. The surface of NPs has a major contribution in their high reactivity. Modification of NPs surface by dyes (which enhance induced photodynamic effects of NPs), or thiols (antioxidant protectors) can completely change the properties and biological effects of NPs.

RE-based NPs with different form-factor and size were used: spherical - $GdYVO_4:Eu^{3+}$ (1-2nm), CeO_2 (1-2nm and 8-10nm), spindle - $GdVO_4:Eu^{3+}$ (25 × 8nm), rod-like - $LaVO_4:Eu^{3+}$ (57 × 6-8nm). NPs and their complexes with methylene blue organic dye or glutathione (GSH) adsorbed on their surface were investigated by luminol-dependent chemiluminescence (ChL) in model system of Fenton stimulated reaction and in liver homogenates. UV-induced effects on NP and their complexes also were investigated.

Unmodified spherical $GdYVO_4:Eu^{3+}$ NPs in contrast to the model system have demonstrated prooxidant properties (increase of the light sum and first maximum of ChL) in homogenate. The modification of these NPs with methylene blue enhances UV irradiation effect. Spindle, rod-like and CeO_2 NPs and nanocomplexes with methylene blue have no effect on ChL intensity independently on UV influence. NPs modificated with GSH led to significant decrease of ChL intensity.

Effects of NPs observed in the present study may be ascribed not only to NPs structure but also to processes on the surface of the NP. GSH – dependent mechanisms of NPs influence are discussed.

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TEMPERATURE DEPENDENCE OF THE SURFACE PLASMON RESONANCE IN GOLD NANOPARTICLES

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The temperature dependences of energy and width of the surface plasmon resonance were studied for gold nanoparticles with sizes 20 – 55 nm in silica host matrix in the temperature range 17 – 915 ^{0}C. The increase of temperature leads to appreciable red shift and broadening of the surface plasmon resonance [1] in Au nanoparticles. The obtained dependences were analyzed within the framework of theoretical model considering the thermal expansion of the nanoparticle, the electron-phonon scattering in the nanoparticle and the temperature dependence of dielectric permittivity of the host matrix. The thermal expansion was shown to be the main mechanism responsible for the temperature induced red shift of the surface plasmon resonance in gold nanoparticles. The thermal volume expansion coefficient for Au nanoparticles was found to be size-independent in the studied size range. Meanwhile, the increase of electron-phonon scattering rate with increasing temperature was shown to be the dominant mechanism of the surface plasmon resonance broadening in the gold nanoparticles.

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CORRELATION BETWEEN MORPHOLOGY, CRYSTAL STRUCTURE AND LUMINESCENCE PROPERTIES OF ULTRADISPERSED $La_{1-x}RE_xVO_4$ POWDERS

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Spectroscopic investigation of light emitting materials based on rare earth orthovanadates is an important research task due to a wide application of such materials for various science and technology purposes. Improvement of their characteristics requires study of related properties of various states of these compounds. Synthesized series of the $La_{1-x}RE_xVO_4$ powders were obtained by solid state, co-precipitation and sol gel methods. Phase compositions and crystal lattice parameters were determined by XRD. The $LaVO_4$ samples possess monoclinic structure, whereas the $La_{1-x}RE_xVO_4$ compositions transform in tetragonal structure at $x > 0.1$. The microstructure of the obtained compounds was studied with SEM. Emission spectra of the investigated samples consist of wide non-structural bands of the matrix emission and narrow spectral lines caused by inner *f-f* electron transitions in the impurity ions for the pure and RE-doped compounds, respectively. Characteristics of the both types of emission depend on method of synthesis, viz. on sizes of the powder grains. The obtained dependencies are discussed using proposed models for matrix emission and structure of the nearest surrounding of the RE^{3+} centers.

Luminescence properties were investigated using excitation with synchrotron radiation at SUPERLUMI station at HASYLAB, DESY, Hamburg, (Project # I-20110592). Some data were obtained using the equipment for spectral-luminescent investigations at R&D Laboratory “Spectroscopy of Condensed State of Matter” of Physics Faculty, Taras Shevchenko National University. The investigation was supported by DFFD of Ukraine (Project # F54/040).

RAMAN SPECTRA OF MULTIWALL CARBON NANOTUBES MODIFIED WITH Ce_xO_y

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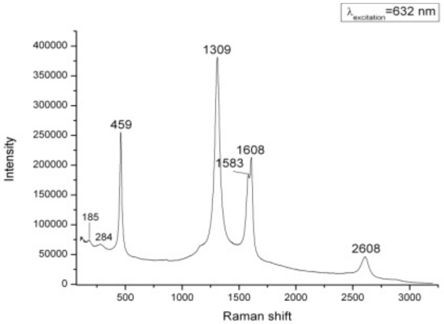
Multi-walled carbon nanotubes (MWCNT) modified by Ce_xO_y (units %) is supposed to be used as catalysts for chemical reactions. That is why we have created and studied this system for conversion of primary alcohol in ketone. Raman spectra (RS) have been registered with Renishaw inVia Raman Microscope in the 100-3200 cm^{-1} region with laser's wavelength of 632 nm and visualized with electronic transmittance microscopy (FEI Tecnai G^2 20 X-TWIN). RS and microscopy certified that nanoparticles of Ce_xO_y localized on the surface of MWCNT and distributed non-homogenously. We have registered mode of CeO_2 near 459 nm (See fig) in this system with the same intensity as G-mode of MWCNT as well with negligible intensity. According to RS data we estimated the size of Ce_xO_y particles in the region of 10-30 nm.



Chemical test showed that our system is effective in catalysis of conversion of primary alcohol in ketone that occur according the dehydrogenization mechanism.

Acknowledgment: we thank for financial assistance Ukrainian-Polish Joint Research Project (2012-2014), PIRSES-2012-318617 FAEMCAR.

FORMATION AND LUMINESCENCE PROPERTIES OF A^2B^6 NANOCRYSTALS IN PORES OF SiO_2 MATRIX

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In this work the luminescence properties of A^2B^6 nanocrystals incorporated in pores of SiO_2 matrices have been investigated. ZnSe nanocrystals were obtained by two different methods: by selenation of SiO_2:$ZnCl_2$ matrices and by chemical vapor deposition (CVD). The spectra of ZnSe nanocrystals in silica pores besides 500 nm band typical for CVD crystal contains broad structureless band in region of 550-700 nm.

All investigations have been performed at 77 K and 300 K. Whereas, intensity of 500 nm luminescence band in CVD crystal strongly depends on temperature and it does not appear at 300 K, any sufficient temperature dependence of SiO_2:ZnSe luminescence is not observed. Appearance of red band at 550-700 nm and absence of temperature quenching indicates strongly coupled localized states formation in SiO_2:ZnSe matrices. These localized states can be ascribed to the SiO_2-ZnSe surface layer [1].

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THE INTERCONNECTION OF PREMELTING PHENOMENON AND NONLINEAR-QUANTUM MECHANISMS OF CANCER DISEASES EVOLUTION

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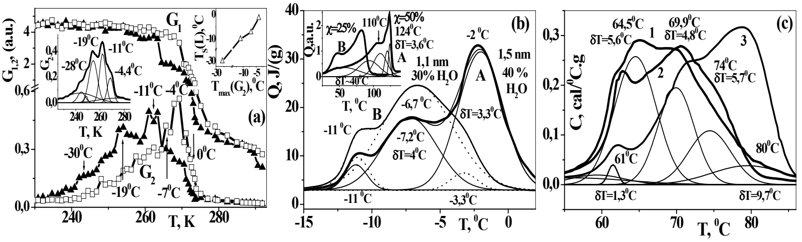
The phenomenon of premelting is known since the times of Faraday, however, nonlinear-quantum and vibrational-electron nature of this phenomenon has been established only in our times [1]. This makes it possible to investigate deep inter-relation between the elasto-viscous properties of ice [1], discrete properties of water nano-films stability at the surface of the ice [2], wide temperature range of water nano-layers and amorphous media melting [3] and the mechanism of evolution of diseases including cancer ones.

Temperature dependencies of the real $G_1(T)$ and imaginary $G_2(T)$ components of the shift modulus of polycrystalline ice are shown at fig.a. One can observe a series of leaps of $G_1(T)$, where the elasticity of ice decreases suddenly, as well as a series of maxima of $G_2(T)$ at temperatures T= -4, -7, -11, -19 and -30°C, where the viscosity increases.The temperatures of maxima T_{max} coincide with temperature ranges of stability Ts of thicknesses of quasi-liquid films L(T) [2] (inset of fig.a).

It is substantial that the values of T_{max} and Ts agree also with the temperatures of maxima of differential scanning calorimetry (DSC) T_{DSC} observed during the melting of nanolayers of ice with thickness of d~0,6÷5 nm in lamellar mesophase (see fig.b). Depending on vibrational-electron interaction (VEI) different scenarios of nanowater and polyethylene (inset) melting exist, which is illustrated with cur-ves A and B on fig.b. This facts can be supported with the results of DSC taken du-ring cancer [4], which are dem-



onstrated on fig.c. On the figure we show endoterms of DSC taken during endometrial cancer (1), lung cancer (2) and lyme disease (3).

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EFFECT OF OXYGEN NONSTOICHIOMETRY ON THE LUMINESCENCE PROPERTIES OF NANOCRYSTALLINE CERIUM OXIDE

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Cerium oxide has found application in different technology fields. Cerium oxide is widely used in protective UV absorbing coatings, as the main component of the polishing compounds, in electrochromic coatings, etc. Antioxidative properties of CeO_2 nanocrystals allow to use this material in the wide range of biomedical applications [1, 2].

Cerium can exhibit both the +3 and +4 oxidation states, and nonstoichiometric oxides can be formed. 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 [3]. 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 different degrees of oxygen nonstoichiometry have been investigated by means of luminescence spectroscopy techniques. It was shown that luminescence of CeO_2 is determined by two optical centers of different nature: the first one - Ce^{4+}-O^{2-} complex and the second one - Ce^{3+} ions. Luminescent characteristics of optical centers 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.

Variation of the Ce^{3+}/Ce^{4+} ratio in CeO_2 allows to control the oxygen nonstoichiometry by luminescence properties of this material. Size dependence of oxygen nonstoichiometry for CeO_2 nanocrystalls was shown.

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FLUORESCENT LABELING OF NANO-SCALE CARRIERS: VISUALIZATION OF NANOCARRIERS – MEMBRANE INTERACTION IN MODEL SYSTEMS AND LIVING CELLS

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In the current studies, a large variety of nanomaterials, such as liposomes, polymeric micelles, quantum dots, magnetic nanoparticles, compounds activated by rare earth elements, fluorophore-tagged latex/silica nanoparticles, fluorophore–labeled polymeric nanospheres etc. are used as fluorescent probes and labels. Strong interest in such objects is dictated also by the fact that nanoparticles have the potential to revolutionize the diagnosis and treatment of many diseases, for example cancer and infectious diseases. Liposomes and the nanoparticles with sizes ranging from a few tens to hundreds of nanometers are used for targeted delivery of active substances. Medicines can be incapsulated in the lipid bilayers of the liposomes or adsorbed on the nanoparticle's surface.

The target delivery of active substances is carried out by the mechanism of passive or active transport. For example, nanoparticles with sizes less than 300 nm accumulate in tumor tissues with a developed circulatory system due to the enhanced permeability and the retention effect [1].

In the present study, fluorescence labeling was based on the phenomenon of fluorescence resonance energy transfer (FRET) between several dyes encapsulated in nano-scale volume. Inorganic anionic nanoparticles (nGdYVO4:Eu^{3+}, d = 2 nm, CeO$_2$, d = 2nm) and phosphatidylcholine liposomal vesicles have been used as nanocarriers. Organic cationic dyes from carbocyanine family (DiOC$_{18}$, DiIC$_{18}$, DiDC$_{18}$) have been used as a model system of the active substance. The dynamics of dyes release as the result of nanocarriers interaction with the model of cell membranes and rat hepatocytes was analyzed based on FRET signal redistribution in time. The significant differences in the dyes release dynamics has been revealed depending on the nanocarrier type. The way to control of the active compound release is proposed.

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TEMPERATURE DEPENDENT SURFACE PLASMON ENHANCED PHOTOLUMINESCENCE FROM SILVER NANOPARTICLES

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The temperature dependence of the photoluminescence (PL) from spherical silver nanoparticles having the size in the range 8 – 30 nm embedded in a silica host medium was studied experimentally in the temperature interval 78 – 298 K. The PL spectra of Ag nanoparticles having two-band structure were rationalized as the result of radiative interband transitions enhanced by the coupling of exciting and emitted photons to surface plasmon resonance excited in the nanoparticles. The quantum yield of PL from silver nanoparticles was found to increase when the temperature decreased. Such temperature dependence was explained as the result of increase of the plasmonic enhancement factor with decreasing temperature occurring due to decrease of electron-phonon scattering rate. The theoretical calculations of the temperature behaviour of PL spectra from silver nanoparticles agree well with the results of experimental observations proving the above assumption. We observed that temperature dependences of PL quantum yield are stronger for small nanoparticles. This effect was shown to be caused by the dependence of the strength of electron-phonon coupling in the silver nanoparticles on their size. The strength of electron-phonon coupling increases in 2.3 times when the nanoparticle size decreases from 30 to 8 nm.

RAMAN SPECTRA OF THE PARATELLURITE CRYSTALLIZED IN NANOSCALE SYNTHETIC OPAL PORES

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The synthesis of predisposed to polymorphism active dielectrics in restricted nanoscale space attracts considerable attention due to possibility of obtaining the existing polymorphous modifications and study their physical properties.

The objective of this work is to research the vibrational and structural properties of TeO_2 crystals grown in nanoscale synthetic opal pores with using Raman spectroscopy technique.

Filling of the synthetic opal pores with the average linear size of 70 nm was carried out by melting-in of α-TeO_2 fine-dispersed polycrystalline powder.

Raman spectra of prepared samples and fine-dispersive powder were measured on a laser spectrometer on basis of DFS-12 with use DPSS laser (λ = 532 nm, power of 120mW). Registration of the useful signal was carried out in the [111] direction.

The studying of Raman spectra of prepared samples has allowed to establish that substance inside opal pores is in the crystalline state and the structure is very sensitive to crystallization regime. Furthermore, the obtained Raman spectra were compared with the α-TeO_2 polycrystalline powder spectra and single crystal spectra in different polarization geometries for the making of a comparative analysis. Due to performed analysis a new line 430 cm^{-1} and significant gain of line 685 cm^{-1} was found in Raman spectra of samples. Taking into account the results in [1] was made the conclusion that these changes are caused by manifestation of the tellurium dioxide metastable form (γ-TeO_2) not existing under ambient conditions. As well, the overall enhancement of the Raman spectra, explained by an increase of the light interaction time with substance in the opal template pores was observed.

This work was financially supported by SFFR of Ukraine – RFFR of Russia project “Creation and investigation of active matrix nanocomposites on the base of photonic glasses and crystals for solar cells”.

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MICRO-RAMAN, REFLECTION AND ATR STUDY OF METAL-SEMICONDUCTOR NANOCOMPOSITES BASED ON POROUS III-V SEMICONDUCTORS

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New material - metal-semiconductor nanocomposite based on well-ordered InP porous layers have been investigated. Different photo-physical phenomena can be enhanced in such media due to excitation of the local (surface) modes in the metal inclusion and further energy transfer to the environment. This fact makes the material promising for photonics, sensorics or as substrates for Raman scattering measurements. Porosity has been electro-chemically created. Metal inclusions have been incorporated into the pores by the two methods: with use of previously synthesized particles or from an aqueous solution of the Au salt in an electrochemical cell. Diameter of pores was in the range 50 - 200 nm and metal particle size was in 10-40 nm range. Optical properties were studied by micro-Raman mapping (using NTEGRA Spectra system in an upright configuration), specular reflection and ATR (spectral complex KSDI-82) in the phonon range of the semiconductor, i.e. in far-IR spectral region. As found, phonon band intensities are significantly increased in the porous region. The homogeneity of the porous layers prepared has been reliably proved by the Raman micro-spectroscopic mapping of their fresh cleavages. Incorporation of gold nanoparticles into InP layer pores leads to an significant enhancement of the Raman signal from TO and LO modes, especially in the two-phonon band region, also surface phonon polariton mode arise.

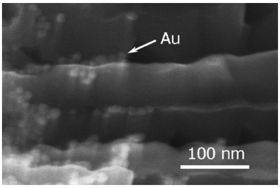

Fig.1. SEM image of the cross section of nanocomposites layer: porous InP with spherical gold nanoparticles in the pores.

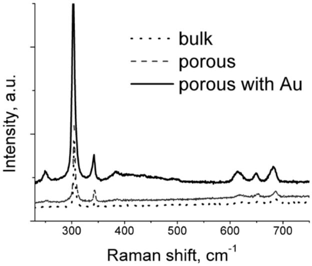

Fig. 2. Raman scattering spectra of the InP samples.

THE KINETICS OF GAS SORPTION BY BUNDLES OF SINGLE-WALLED CARBON NANOTUBES. QUANTUM EFFECTS

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The low temperature kinetics of sorption of ^{3} He, ^{4}He, H_2, D_2, Ne and N_2 gases by bundles of single-walled carbon nanotubes with closed ends (c-SWNT) and the subsequent desorption of these gases from the c-SWNT bundles has been investigated. The characteristic times of the sorption-desorption processes coincide within the experimental error. The prior annealing of the SWNT samples at T=500 C reduced significantly the characteristic times and changed their temperature dependences. The effect of annealing decreased at the molecular weight of the dissolved gas was increasing. Below 16 K the times of ^{3}He, ^{4}He, H_2, D_2 sorption were only slightly dependent on temperature, which suggests a tunnel character of the sorption of these impurities by c-SWNT bundles. The influence of irradiation of c-SWNT bundles with γ-quanta upon H_2 sorption [1] is qualitatively similar to annealing effect.

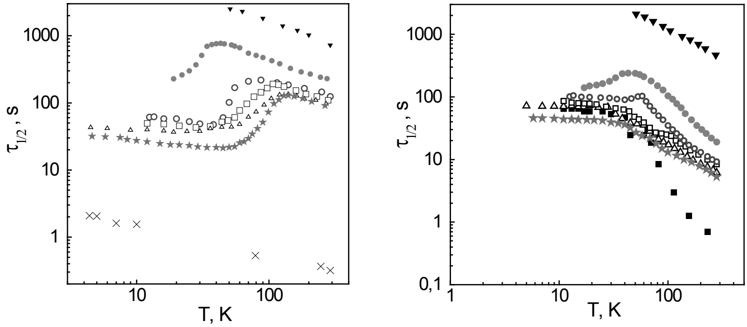

Fig. The temperature dependences of the characteristic times of gas sorption (a) by the starting SWNT sample without a preliminary thermal treatment, (b) by a SWNT sample after heating in vacuum to 500 C (asterisks - ^{3}He, empty triangles – ^{4}He, empty squares – H_2, empty circles – D_2, solid circles – Ne, solid triangles – N_2). Solid squares (b) show the characteristic times of H_2 sorption by a SWNT sample irradiated with γ-quanta in the hydrogen atmosphere.

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TEMPERATURE DEPENDENCE OF THE SURFACE PLASMON RESONANCE IN SILVER NANOPARTICLES

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The temperature dependences of energy and width of the surface plasmon resonance were studied for silver nanoparticles with sizes 24 – 60 nm in silica host matrix in the temperature range 17 – 700^{0}C. The increase of temperature leads to appreciable red shift and broadening of the surface plasmon resonance [1] in Ag nanoparticles. The obtained dependences were analyzed within the framework of theoretical model considering the thermal expansion of the nanoparticle, the electron-phonon scattering in the nanoparticle and the temperature dependence of dielectric permittivity of the host matrix. The thermal expansion was shown to be the main mechanism responsible for the temperature induced red shift of the surface plasmon resonance in silver nanoparticles. The thermal volume expansion coefficient for Ag nanoparticles was found to be size-independent in the studied size range. Meanwhile, the increase of electron-phonon scattering rate with increasing temperature was shown to be the dominant mechanism of the surface plasmon resonance broadening in the silver nanoparticles.

[1]. O. A. Yeshchenko, I. M. Dmitruk, A. A. Alexeenko, A. V. Kotko, J. Verdal, A. O. Pinchuk, Plasmonics (2012) DOI: 10.1007/s11468-012-9359-z.

ENHANCEMENT OF ELECTRON-HOLE GENERATION RATE BY METAL NANOWIRE ENSEMBLE NEAR SEMICONDUCTOR SUBSTRATE

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Enhancement of electromagnetic field intensity in thin semiconductor films is very important for many applications in nanophotonics, optoelectronics, sensorics and photovoltaics. The extraordinary light transmittance into semiconductor base of nanophotonic or photoelectric devices due to light trapping via excitation of surface plasmons in metal nanoparticles, nanowires and surface plasmon polaritons in periodical array of these particles (wires) on the front surface of semiconductor base is possible [1,2].

Thus, in this report the effective light trapping via presence of the 1D periodic array of metal nanowires at various distance from semiconductor substrate with planar surface was analyzed theoretically. Theoretical calculation of light transmittance/reflectance and generation rate of electron-hole pairs due to excitation of surface plasmons and surface plasmon polaritons has been fulfilled in the framework of curvilinear transformation method. All spectral data for transmittance/reflectance and generation rate are non-monotonic with peak-like shape. The position of peak is the same for all spectral dependencies and is related to local plasmon excitations in nanowires. It was found that the scattering of light by the 1D periodic array of gold nanowires with cylindrical cross section leads: i) to increasing of electron-hole generation rate in semiconductor base and ii) there is optimal distance for which this enhancement is maximal. For example, for gold cylindrical nanowire ensemble with diameter 100 nm and 760 nm period the optimal distance from GaAs substrate is about 100 nm.

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IR-SPECTROSCOPY INVESTIGATION OF Ni/NiO NANOPOWDERS FORMATION DURING THERMAL DECOMPOSITION OF NICKEL ACETATE AMINES

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Ni/NiO nanopowders with different particle size have been synthesized using thermal decomposition of nickel acetate ammines in air at 400 °C for 10 to 180 min.

At the first stage of thermal decomposition of nickel ammine complexes water solutions initial complex lost ammonia and water excess. This stage accompanied with formation of coordinating bonds of nickel-ion with water and acetate-ion.

The next decomposition led to following water loss and acetate-ion decomposition to carbonate beginning. Attenuation of adsorbed water O-H valent oscillation and acetate C-H bond valent oscillation was evidence of this fact. Disappearance of acetate-ion and nickel Ni-O bond valent oscillation authenticated that intermediate nickel complexes with acetate had low stability. In addition, attenuation of N-H bond valent symmetric and valent asymmetric oscillation occurred without attenuation of Ni-N valent oscillation and NH_3 deformative oscillation. This authenticated that bound-free ammonia lost without nickel ammonia water complex composition changing. After 20 min annealing scarcely full acetate decomposition was observed. Disappearance of coordinated water HOH group deformative oscillation at 1620 – 1630 cm^{-1} evidenced of intermediate nickel ammonia water complex full dehydration to nickel ammonia hydroxide complex formation. In addition, Ni-O bond valent oscillation of nickel oxide at 460 cm^{-1} appeared in IR-spectra.

The next decomposition led to full nickel acetate ammines conversion into Ni/NiO phases mixture but full ammonia removing from products didn't observed. Partial coordinated ammonia removing form system occurred gradually in several stages. This process accompanied with nitrate-ion and water formation on power surface. Nitrate-ion formation on power surface authenticated ammonia oxidation by air oxygen or/and for account of nickel oxide reduction to metal nickel. Nickel oxidation by air observed after annealing during 1 hour.

A ROLE OF POLYMER CHAIN RIGIDITY IN THE FORMATION OF STABLE NANOTUBE-RNA NANOHYBRIDS

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Nanotechnologies employ the unique properties of nanoscale materials for the development of modern sensing systems. Carbon nanotubes are suitable for this goal due to their extraordinary physical properties. Biopolymers conjugated with SWNT facilitate their application in advanced technology. Present-day efforts have focused on combining the two in order to incorporate useful properties of each into a single, multifunctional biopolymer-carbon nanotube hybrid.

We have studied the adsorption of two homopolynucleotides poly(rI) and poly(rC) with different chain rigidities on SWCNT, employing UV VIS absorption spectroscopy with analysis of absorption spectra of the hybrid aqueous suspension at room and high temperatures, and MD simulations that explore mechanisms of spontaneous oligomer adsorption on the nanotube surface and energetic properties of SWCNT:$r(C)_{25}$ and SWCNT:$r(I)_{25}$. We showed that adsorption of the poor base stacked poly(rI) onto the nanotube in aqueous suspension is less effective than that of the high base stacked poly(rC) the chain of which is of higher rigidity. Heating of the nanotube:polymer aqueous suspension to 90 ^{0}C, which leads to partial nanotube aggregation and precipitation because of weak bounded polymer sliding from the tube surface, revealed that a part of aggregated nanotubes is about 2.3 larger for SWCNT:poly(rI) suspension than for SWCNT:poly(rC). This fact indicates the higher stability of SWCNT:poly(rC) hybrid in comparison with SWCNT:poly(rI). Less effective adsorption of poly(rI) is confirmed with a weaker hypochromic effect of nanotubes covered with poly(rI) than with poly(rC), which originates from π-π-stacking of nitrogen bases with the nanotube surface.

MD modeling demonstrated that oligomer $r(I)_{25}$ has an essentially weaker energy of binding to the carbon nanotube surface than $r(C)_{25}$ (250 kcal/mol vs. 325 kcal/mol). Difference in energies of binding to the tube surface is explained with a smaller number of nitrogen bases of $r(I)_{25}$ π-stacked with the tube surface than $r(C)_{25}$ (13 vs 19).

NONLINEAR EFFECTS OF THE LATERAL PHOTOCURRENT IN InGaAs/GaAs QUANTUM DOT STRUCTURES

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In this paper we studied the spectra of the lateral photoconductivity (LPC) and dependence of LPC on incident light excitation power density in multilayer $In_{0.4}Ga_{0.6}As$/GaAs heterostructures with quantum dots (QDs) and influence of the radiative recombination on the photosensitivity of the QD arrays and defects. Explanation of the mechanisms of nonequilibrium processes associated with the defect states and the photocurrent nonlinearities will give more complete understanding of the optical properties of heterostructures and hence the possibility of a wider use of it.

Particular attention is paid to the impact of the processes of generation and recombination at photosensitivity of the deep defects and QD arrays. It is found a significant effect of radiative recombination on the shape of the LPC spectra. Recombination leads to a nonlinearity of the dependence of photocurrent on excitation power density: when power density is “low”, and hence number of excited electron-hole pairs is small, the process of radiative recombination of charge carriers in the QDs is prevail over their generation. It helped open the question of why the ionization spectrum of defects, including levels EL2 and EB3, has not typical for this kind of spectra a sharp decline in excitation energy where absorb nanoscale $In_xGa_{1-x}As$ layers.

The nonlinear dependencies of the LPC on power density of incident light excitation are study. For the component of the spectrum, which corresponds to the photocurrent from the QD ground state (1.23 eV), the nonlinear dependence of the LPC on excitation power density is explained as competition of processes of the generation and thermal activation on the one hand and the radiative recombination on the other. Number of free charge carriers in the conduction barrier layers is small in relation to the number of possible centers of capture (quantum wells of QDs and defect traps) at low excitation intensity, consequence the radiative and non-radiative recombination overwhelm over generation, but further increasing of the excitation power density caused the increasing of the density of free charge carrier and as a result the impact of recombination on photocurrent becomes less noticeable. The observation of nonlinear phenomena of photocurrent at 1.34 eV incident light excitation is due to the presence of both local electric fields at the $In_xGa_{1-x}As$/GaAs interface caused by structural non-uniformities and a traps below the GaAs conductivity band edge.

RAMAN AND ION BEAM MICROSCOPY IMAGING OF NANOMATERIAL TRANSLOCATION IN THE BIOLOGICAL ENVIRONMENT

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The degree and the mechanism of uptake, localization and distribution of NPs in cells and organs are major issues concerning toxicity and risk assessment of these novel products. Furthermore, the application of NPs as devices for diagnostic and therapeutic purposes requires monitoring of their interaction with cells. Label-free imaging techniques, which allow studying authentic nanoparticles and nanomaterials within their biological environment, are therefore required.

Confocal Raman Microspectroscopy (CRM) and Ion Beam Microscopy (IBM) are especially suitable. They are label-free techniques capable of detecting and characterizing nanomaterials within single cells. The uptake, intracellular distribution and toxicity of metal oxide nanoparticles, surface modified carbon nanotubes (CNTs) in hepatocarcinoma and lung cells (A549) were studied employing these techniques. By means of IBM the intracellular concentration and distribution of NPs can be established. This provides the basis for intracellular dose dependent toxicity studies.

By means of Raman spectra deconvolution and subsequent cross-correlation analysis the co-localization of NPs with different intracellular environments, such as lipid rich regions, cytoplasm and nucleus was quantified. CRM, furthermore, was capable of detecting nanomaterial-induced changes in the secondary nuclear protein structure and nucleobase content. These changes can be used as an indicator of the toxic effect of NPs. This was confirmed with cell proliferation tests. Studies with NPs surface engineered with lipids and polyelectrolytes showed that the nature of the surface of NPs is crucial for uptake and toxicity.

MANIFESTATION OF STRUCTURE OF ELECTRON BANDS IN DOUBLE-RESONANT RAMAN SPECTRA OF ONE- AND TWO-LAYER GRAPHENES, BULK GRAPHITE AND SINGLE-WALLED CARBON NANOTUBES

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Resonance micro-Raman spectra of one- and two-layer graphenes, bulk graphite crystals and mixture of single-walled carbon nanotubes (SWCNTs) in the range of two-phonon 2D bands were in details experimentally investigated. The fine structure of these 2D bands in the investigated carbon allotropes is considered as been caused by the structure of their pi-electron zones.

The theory-group classification of involved in electron-phonon resonances electron and phonon states is carried out according to projective irreducible representations of wave vector groups. In particular, the vibration states of bulk graphite in A-point of Brillouin zone and SWCNTs in boundary A_K and A_M points of one-dimensional Brillouin zone were shown to transform according to one-valued representations of projective class K_5, and their electron states – according to two-valued representations of projective class K_4. The compatibility relations characterizing the dispersion of vibrational and electronic states for Γ-A directions were constructed. The nature of the doublet behavior of phonon 2D bands in graphite bulk crystals is related with double electron-phonon resonance involving phonons participating in intervalley electron transitions and in SWCNTs – with phonons participating in intravalley electron transitions. To confirm these mechanisms the forms of vibrations for these specified phonons are also analyzed.

LASER–INDUCED EXCITONIC LUMINESCENCE OF NANOCRYSTALLINE TiO_2 POWDERS

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The optical absorption and photoluminescence of nanocrystalline anatase and rutile TiO_2 are studied at room temperature. TiO_2 powders were synthesized in the form of pure anatase or rutile. The samples are characterized by X-ray diffraction, X-ray fluorescence, Raman spectroscopy, optical absorption and photoluminescence (PL) methods. The room-temperature PL spectra are studied under the intensive UV (3.68 eV) N_2-laser excitation. Some interesting features in the PL spectra including the well-resolved peaks of excitonic and band-to-band transitions in TiO_2 are observed for the first time. It is shown that PL bands including peaks at 2.71-2.81 eV and their phonon replicas in anatase and rutile TiO_2 arise from the excitonic e^--h^+ recombination via oxygen vacancies. The excitonic peak at 2.91 eV is attributed to the recombination of self-trapped excitons in anatase, or free excitons in rutile TiO_2, respectively. The PL peaks within 3.0-3.3 eV in anatase TiO_2 are ascribed to indirect allowed transitions due to band-to-band e^--h^+ recombination. The peaks at 3.03 eV and 3.26 eV are attributed to free exciton emission near the fundamental band edge in rutile and anatase TiO_2, respectively. The influence of TiO_2 crystal structure and calcination temperature on the PL spectra is discussed.

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RAMAN SPECTROSCOPY OF FULLERENE FILMS IN THE TEMPERATURE RANGE 5 – 300 K: THE SPECTRA PECULIARITIES NEAR THE STRUCTURAL PHASE TRANSITION

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Raman spectroscopy is an informative method at the study of the structural phase transition (SPT) observed in the solids. Earlier this method was exploited to study the SPT in the single-crystals of C_{60} [1]. The purpose of this work is a study of the SPT influence on Raman spectra of polycrystal unpolymerized and photopolymerized films deposited on the silicon substrate.

At temperature lowering from room to 250 K the peak of the line corresponding to $A_g(2)$ mode in unpolymerized film of C_{60} is up-shifted monotonically (~ 1.0 cm^{-1}). At a further temperature lowering (to 5 K) the value of peak frequency of this line decreases (~ 1.5 cm^{-1}). Such temperature dependence of peak position of this line differs from the dependence observed before for the single-crystal of C_{60} [1], for which at temperature decreasing below 252 K (SPT) the peak of this line is up-shifted. A difference in temperature behavior of this line of polycrystal unpolymerized film and single-crystal of C_{60} is discussed.

The temperature measuring of photopolymerized fullerene film showed absence of anomaly in the frequency behavior of the lines at the temperature near the SPT. In these films the position of lines, corresponding to $A_g(2)$ mode of monomers, dimers, linear chains and trimers is up-shifted monotonically on ~ 1.5 cm^{-1} at a temperature decrease from 300 to 5 K.

For polycrystal unpolymerized fullerene film in range of A_g and practically all H_g modes the splitting of lines is found out at low temperatures which was before observed only in single-crystals. This splitting is caused by both the lowering of symmetry of free molecule of C_{60} in the crystalline field and by appearance of additional components in a low temperature phase as a result of the SPT at which the unit cell value is increased in four times. For photopolymerized fullerene film the similar line splitting is not observed.

The process of photopolymerization of the fullerene film is studied for polycrystal unpolymerized fullerene film under argon laser irradiation at temperatures higher and below than temperature of the SPT.

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PHOTOINDUCED CONDUCTIVITY CHANGES IN Ge-NC/SiO_2/Si STRUCTURES: PERSISTENT AND QUENCHING EFFECTS

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Two optically induced steady-states with excess and shortage of surface conductivity values as compare to equilibrium one were observed in structures with Ge NCs grown on silicon oxide at low temperatures. Result of photoinduced changes depends on photon energy due to different type of electronic transitions observed in Ge-NC/SiO_2/Si structures. The persistent photoconductivity behaviour was observed after excitation of electron-hole pairs in Si(001) substrate due to interband absorption in Si. The conductivity excess may be attributed to spatial carrier separation by macroscopic fields in the depletion layer of near-surface Si. Interband transitions in Ge creates localized holes in Ge directly, leading to optically-induced spatial redistribution of trapped positive charges between SiO_2/Si interface levels and localized states of Ge-NCs, which enhance variation of electrostatic potential in underlying Si and, therefore, decay of surface conductivity under stationary photoexcitation. Observed results demonstrate that hole trapping by Ge-NCs and interface states have significant on in-plane transport in the Ge-NCs/SiO_2/Si structures. Observed possibility for optically-control switching between different modes of system's conductivity may be helpful for design optical memory devices.

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STRENGTHENING OVERTONES AND COMBINATION TONES IN THE VIBRATIONAL SPECTRA OF TiO_2 NANOFIBERS AND NANOFILMS AND THEIR COMPOSITES WITH NANOPARTICLES OF Au, Ag AND CARBON NANOTUBES

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TiO2 nanofilms (~ 200 nm thick) with anatase phase were synthesized by sol-gel method on the surface of crystalline silicon and anatase nanofibers diameter of 10-20 nm were synthesized by hydrothermal synthesis. A comparative study of the Raman spectra (488 nm) of anatase microcrystals, nanofilms and nanofibers was shown in Fig. a. In this case, the spectra were normalized to the maximum of the most intense vibrational band (VB) ν_1 = 143 cm^{-1}. A thorough computational processing was maden for broadband background as the main vibrational bands ν_1-5 and second and third order bands (insert). It was shown that in a number of microcrystals (1)-nanofilm (2) -TiO_2 nanofibers (3) overtone $2\nu_1$ band maximum increases by more than 15 times, and the difference tones ν_4-ν_3 (ν_5-ν_4) and ν_5-ν_3 (ν_3-ν_1) become stronger ~ 30-50 times (Fig.b). This indicates a strong increase of the vibrational anharmonicity and nonlinearity in nanostructures. Simultaneously there is a broadening of the observed vibrational bands in 1.5-4 times. As a result, the integral intensities of the second order bands increase in 30-200 times.

The nonmonotonic dependence of the intensities of VB ν_1, ν_3 = 396 and ν_5 = 637 cm^{-1} on the dose of Ti^+ ions (140 keV) were found for TiO_2 nanofilms (inset Fig.b). At low doses D = 10^{12}-10^{13} ions/cm^2 intensity of VB increase ~ 1.5 times, which is associated with improved of material properties and for D>10^{14} ions/cm^2 VB attenuated. For TiO_2 nanofilms with Au, Ag nanoparticles (d=10-20 nm) is observed more weakening of VB at high D. It is essential that the reduction of VB with D increasing is accompanied by a significant increase in the induced electron bands, due to the strong vibration-electron interaction (VEI). It is shown that the growth of the intensities of VB dominated VEI, and the influence of plasmon resonance is not the main one. VEI is associated with the nonlinear resonant interaction of VB. The vibrational resonances $\mathbf{2\nu_2=\nu_3}$, $\mathbf{2\nu_4\approx\nu_3+\nu_5}$ and $\mathbf{2\nu_3\approx\nu_1+\nu_5}$ of TiO_2 contribute to enhancement of nonlinearity.

For TiO_2 nanofibers with multi-walled carbon nanotubes (CNT) the bands of overtones and combination tones are enhanced even further, indicating that the strengthening and growth of VEI and vibrational nonlinearity. It proved by a significant strengthening and broadening of the D and G bands of CNT with frequencies 1360 and 1585 cm^{-1} after annealing at 600^0C (1 hour) (Fig.c). This contributed significantly to the total resonance tones $\mathbf{2\nu_3+\nu_5}$ and $\mathbf{2\nu_4+\nu_5}$ nanofibers with D and G bands of CNT (insert fig.c).

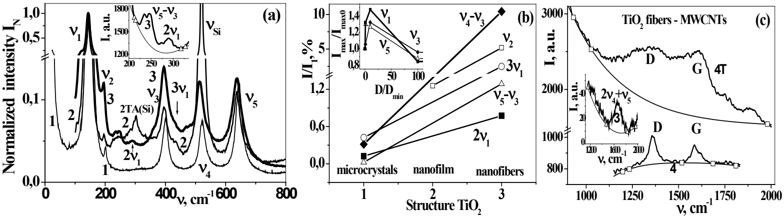

Fig.1. A comparison of the Raman spectra of the microcrystals (1) nanofilms (2) nanofibers and (3) of anatase (a), increase in bands of overtones and difference tones in nanostructures and nonmonotonic doses dependence of bands $\mathbf{\nu_{1,3,5}}$ intensively of anatase nanofilms (insert) (b), and increase and broadening of D and G bands of MWCNT in nanocomposites with TiO_2 nanofibers annealing at 600^0C (c).

ENHANCEMENT OF ACTIVE AND «SILENT» VIBRATIONAL BANDS IN RAMAN AND IR SPECTRA OF C_{60} NANOFILMS

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By comparing the Raman and IR absorption spectra of nanofilms (NF) with thickness d = 150-250 nm and microfilm (d = 1,2-2 mm) of fullerene C_{60} a large gain the intensities of the Raman-active vibrational bands (VB) Hg(1-8) of NF, that for Hg(3,4) bands shown in the inset (Fig.1a). This is shown in Fig.la for the ratio of the maximum of Raman bands Hg(1-8) and Ag(1) for the hot (2) and cold (3) the deposition film methods. Thus, all the spectra were normalized to the strongest Raman and IR lines Ag (2) and F1u (1) with the frequencies 1469 and 527 cm^{-1}. From Fig.1a one can see that the band Hg (1-8) in nanofilms C_{60} amplified 2-7 times compared with the microfilm 2μm. After polymerization of 1 and 2 NF by diamine N_2H_4 (film 1p and 2p) observed the IR VB enhancement becames weaker, which is associated with a decrease in the vibrational nonlinearity.

Enormous enhancement in IR spectra a number of inactive for icosahedral symmetry I_h Hu(2,4), Gu(2-4), Gg(3), F1,2g (1) vibrations in NF (2) in compari-sion with 1.2 μm microfilm (spectrum 1a) is shown in Fig.1.b. The majority bands in the IR spectra of nanofilms increased 5-20 times as shown in the inset Fig1.b. A still greater increasing ~ 50-300 times observed for many of the "silent" vibrations in the Raman spectra of C_{60} nanofilms. The observed anomalous enhancement of the vibrational bands in nanostructures associated with a significant change in the electro-physical properties of nanostructured media as a result of the weakening of symmetry and increased anharmonicity and nonlinear interaction of vibrational modes.

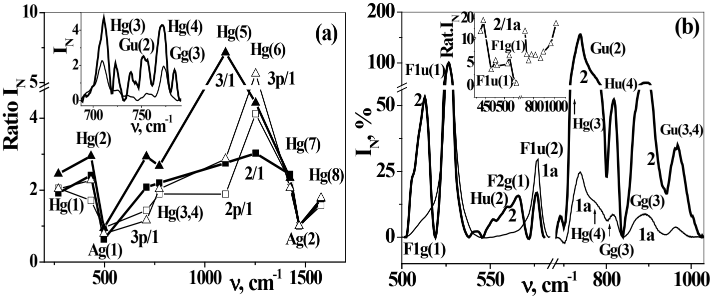

Figure 1. The fragments of enhanced Raman (a) and IR (b) spectra of nano- and micro-films of C_{60}.

STRONG ELECTRON-VIBRATION INTERACTIONS AND INDUCED ELECTRONIC STATES IN NANO- AND MICROFILMS OF FULLERENE C_{60}

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Previously, we have established the electronic nature of the broadband background in the Raman spectra and proved the importance of strong vibration-electronic interac-tions (VEI) [1]. The increasing role of VEI is associated with increased nonlinear resonant interaction of vibrational modes in nanostructures. The efficiency of nonlinear processes in nanofilms of C_{60} abnormally increases due to a number of successive vibrational resonances of the Hg (1)+Hg (2)=Hg (3), 2Hg (3)=Hg (7) [2], the number of which exceeds one hundred and change of electronic states (ES). By examining the Raman spectra (λ_L=514,5 nm) nano- (150–250 nm) and micro-films (1–2 μm) of the fullerene C_{60} we studied in detail the change of induced ES in the band gap, as shown in Fig.1a,b. For nanofilms (NF) the Ag(1) line at 497cm^{-1} observed as well as line ν_{Si} = 520 cm^{-1} of crystalline silicon (inset Fig.1a). In cold deposition process of NF prepara-tion (spectrum 2) the ES bands are several times greater than in films fabricated by hot process (spectrum 1). In the original films 1 and 2 the low-frequency part of the ES is dominated, and after polymerization by N_2H_4 (1p and 2p spectra) ES intensity increases with frequency ν. With sharp focusing of ecitation λ_L electronic bands (EB) are ampli-fied more than 100 times. In addition to broadband ES with half-widths δν ~ (1-2)10^3 in the vinicity of vibrations some “islet” EB with δν ~10^2 cm^{-1} are observed which is shown in the inset Fig.1.b for the vinicity of Hg (3,4) vibration. The non-monotonic dependence on the thickness of the broad EB have been detected in NF which is shown in Fig1,b. The intensity dependence of EB I_0 at 520 and 1470 cm^{-1} in comparing with line intensity ν_{Si} have been done. Reducing I_0 for thin NF due to insufficient accumula-tion of nonlinear wave processes. The role of the strong VEI is also confirmed by the linear weakening of the intensity of the Ag (2) band with increasing I_0(1470 cm^{-1}), as shown in the inset in Fig.b.

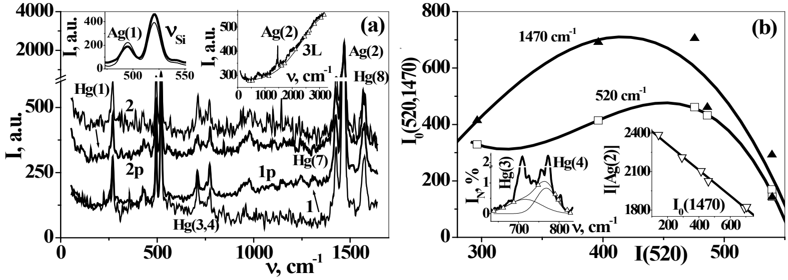

Fig1. The new EB in Raman spectra of C_{60}-nano-films (1,2) and after their polymerri-zetion (1p, 2p) and the strong focusing of the laser excitation (3L) (a) and non-mono-tonic change in the EB intensity I_0 in comparing with the line intensity ν_{Si}=520 cm^{-1} (b).

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EFFECT OF ULTRASOUND FIELDS ON THE OPTICAL PROPERTIES OF FULLERENE FILMS

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Effect of ultrasound propagating in the glass substrate-fullerene film structures on the optical transmission spectra was studied. The changes in the transmission spectra of C_{60} and C_{70} fullerene films at ultrasonic load were investigated. The samples were formed by the vacuum thermal evaporation of C_{60} and C_{70} fullerenes on the glass substrates. Thicknesses of all fullerene films were about 100 nm.

MAGNETO-INDUCED ANISOTROPY OF AN AQUA SUSPENSION OF SUPERPARAMAGNETIC MAGNETITE NANOPARTICLES

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Our recent studies showed a strong magneto-optical response of the aqua suspension of the vanadium pentoxide nanorods doped with quasi-spherical magnetite both for isotropic and nematic phase [1]. To explain the results obtained in [1] we associated the magnetic sensitivity of such suspensions with formation of anisotropic structures – presumably, chains of magnetite nanoparticles by the magnetic field. Here we report on the studies of the effects of magneto-induced birefringence and anisotropy of magnetic susceptibility in the aqua suspension of magnetite nanoparticles, which support this idea.

[1]. S. Kredentser et al. Soft Matter, 2013.

ELECTROREFLECTANCE SPECTROSCOPY OF THE FILM AND FILM-SUBSTRATE INTERFACE IN $Si_{0.75}Ge_{0.25}/Si$ HETEROSYSTEMS

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Heterosystems with SiGe films on Si substrate arise to a great scientific attention due to theirs application in novel technologies and researchers. Their physical properties determined by the composition of the films. During the manufacturing of heterosystems, the internal mechanical stresses appears due to the difference of lattice film and substrate periods and coefficients of thermal expansion. The appearance of mechanical stresses leads to bending of the heterosystems, and accompanied by the structural defects at the interface film-substrate, and reduced the reliability of the devices. An investigation of the electron and optical properties of heterosystems is importance for the technology development and for the prediction of the devices properties.

$Si_{0.75}Ge_{0.25}$ films on Si substrate was obtained by CVD method and had single crystalline structure. Their thickness was 100 nm. The heterosystems were studied by electroreflectance modulation spectroscopy and by profilometry measuring of the heterosystems bending radius. The electroreflectance spectra were measured by an electrolytic method in the spectral range 2.6…3.6 eV. Important data were obtained about the film and interface band structures, their structure perfection, electron parameters (forbidden gap width, conductivity type, the charge carries scattering, the mobility and the time of the energy relaxation of light exciting charge carries) and about the elastic stresses, as well as the influence on them γ- irradiation with dose $10^6…1{,}9\cdot10^7$ R.

As the dose increased, the electron parameter of film and of interface was improve, mechanical stresses decreased. They disappear at the dose $1.5\cdot10^7$ R. At this dose the film changed the composition with the formation of the other solid solution structure. The additional peaks appeared in the spectra of the film. They corresponded to the composition x: 0.8, 0.67, 0.58 and 0.48. The possibility was found to fabrication of the heterosystems without the bending deformation and to improve their electronic properties.

LUMINESCENCE OF THE GOLD FILMS COATED WITH Eu^{3+} CONTAINING ANALYTES

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In this paper the dependences of luminescence intensity of Eu^{3+} ions containing either complexes with CAPh ligands or lanthanum vanadates on morphology of gold films deposited on porous alumina were studied.

Surface enhancement of the light is actively studied for the last two decades and allow observe the spectroscopic properties of single molecules. This feature makes them preferable for modern bio-medical applications.

Compounds based on carbacilamidophosphate (CAPh) ligands as well as lanthanum vanadates are very promising from the various practical approaches particularly resulting from their good biocompatibility.

Nanostructured porous aluminum oxide films were formed by anodic oxidation of aluminum deposited on a glass substrates by magnetron sputtering. Gold nanostructures were made with thermal evaporation in vacuum chamber. Images of surface morphology were made using AFM, ATM and luminescent scanning - microscopy equipment.

Luminescence characteristics of mentioned compounds under photo, X - Ray and VUV excitation, the spectra of their luminescence excitation as well as near field luminescence characteristics were obtained and analyzed.

Experiments with VUV synchrotron radiation were made on SUPERLUMI station, DESY synchrotron, Project I - 20110592. The investigations were supported by DFFD of Ukraine (Project # F54/040) and CNRS - NASU joint project.

SPECTROSCOPIC PROPERTIES OF COMPOSITES, CONSISTING OF 5CB DOPED WITH ORGANOMONTMORILLONITE NANOPARTICLES AND CARBON NANOTUBES

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Doping of liquid crystals with nanotubes (NT) changes abruptly their physical properties. But NT form conglomerates in organic media due to the organophobicity of their surface. To reduce their aggregation ability, we have developed a method of simultaneous modifying the montmorillonite by cetyltrimethylammonium bromide (CTAB) and NT. The bonding is shown to occur due to the adsorption by nanotubes of CTAB alkyl chains on the outer surface of aluminosilicate stacks. Composites with 5CB were produced based on these hybrid particles (OM-NT), and also with only organo-modified montmorillonite (OM) or NT. According to IR-spectroscopy data, narrowing of bands indicates Van-der-Waals interactions between the components, resulting in the alignments of molecules on a phase separation boundary. Photoluminescence of these composites was investigated at room temperature. Doping of inorganic particles lowers emission intensity, its drop depends on the chemical content of particles. Besides, the presence of OM particles is seen in a red-shift of the spectrum, whereas doping with NT or OM-NT leads to a spectral shift towards short wavelengths, being much larger for the latter sample. Opposite behaviours of spectral shifts can be caused by different rearrangements of local electric fields due to the particle insertion in 5CB. Depending on the chemical content, inorganic dopants can increase or reduce an effective dielectric constant, ε, of the 5CB molecule environment, which value is inversely to the exciton binding energy. The OM insulator particles increase ε, resulting in a red-shift of 5CB photoluminescence. Since NT are electroconductive, they lower ε of the system and cause a blue-shift. Larger spectral changes in the case of OM-NT hybrid particles are explained by their homogeneous distribution and percolation network formation in 5CB, proved by polarization microscopy data.

The work was financed by NAS Ukraine, Project VC157.

SERS OF PLASMON-PHONON MODES AT NOBLE METAL NANOPARTICLES

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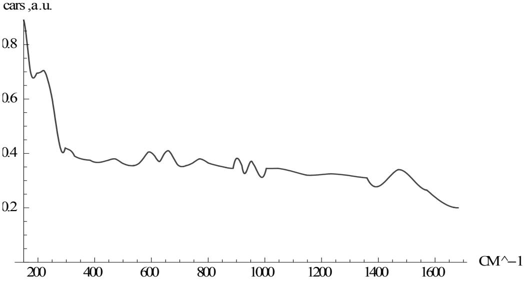
Surface – enhanced Raman spectroscopy (SERS) is efficient method for molecular imaging, molecular diagnostic (including single-molecular sensitivity) [1]. However the lack of signal reproductibility of surface enhancement makes SERS quantitative or semiquantitative in nature. As to our opinion the first step to realize qualitative SERS-method is to use inherent plasmon-phonon mode of SERS as seft referencine standard for the detection and quantification of admolecules. The last will give addition arguments for Raman surface enhancement explanation.

It is well known that several factors contribute to the variation of SERS effeciency: laser wavelength, nanoparticle materials, structure and dimention, enviroment, admolecule concentration, free molecule oscillator spectrum, etc.

All these factors contribute to the surface plasmon exitation by laser wave, local molecule phonon-plasmon interaction and as the result efficiency of resonant Raman scattering at the Fermi resonance of admolecule oscillators modes with surface local phonon modes of metal nanoparticle.

Below we have shown plasmon-phonon band for gold nanoparticles, which are adsorbed on the gold-coated glass slide [2].



One can see that the plasmon-phonon modes spectrum is extented over the thousands cm^{-1}. So it resonantely interects with oscilator modes of adsorbed molecules. The last is due to molecule-nanoparticle adsorption potential, which breaks normal phonon modes structure. We can name that resonant interaction like Fermi-resonance at molecules with low level symmetry.

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[2]. Lan Sun, et al.Biophysical journal (2009), 96, 4709-4716

RAMAN SPECTROSCOPIC CHARACTERIZATION OF NANOGRAPHITE OBTAINED WITH CHEMICAL METHOD

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The work is devoted to Raman spectroscopic investigations of nanographite obtained with chemical method from thermoexfoliated graphite (TEG) and carbon nanotubes (CNT).

The initial carbon materials such as TEG and CNT were treaded with strong inorganic (sulphur and nitric acids, potassium permanganate) and organic (acetone, chloroform, acetone, ethanol and toluene) oxidizers. As the result of such treatment the nanographite structures with small number of graphite layers are obtained. As shown Raman spectroscopic investigations the Raman spectra of all nanographite specimens exhibit two main typical graphite bands: the band at (1581±1)cm^{-1} (G-band) assigned to the in-plane vibration of the C–C bond and the band at (1348-1359)cm^{-1} (D-band) activated by the presence of disorder in the carbon systems. G-band for all nanographite specimens is characterized by high intensity, while the intensity of the D-band is significantly lower. The position of the low intensive D-band arising from the activation in the first order scattering process of sp^3 carbons slightly varies for different specimens. The Raman spectra also exhibit a band around 2700cm^{-1} called the G' band. This band is essentially asymmetric for all nanographite specimens with the peculiar "shoulder" at the low-frequency side. The presence of such "shoulder" indicates the presence of the graphite nanoparticles containing low amount of the graphite planes (<10).

J-AGGREGATES LUMINESCENCE CONTROL VIA INTERACTION WITH SILVER NANOPARTICLES

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In recent years optical properties of various hybrid complexes, for example, organic dyes with nanoparticles of noble metals have been intensively investigated. These systems have a number of unique features. Optical properties of metal nanoparticles are well known and associated with surface plasmon resonance (SPR). SPR phenomenon is widely used for chemical and biological sensors (biosensors) creation. In contact with biological objects (DNA, viruses, antibodies) it allows more than one order increase of the intensity of fluorescence signals.

In present communication we report a possibility for J-aggregate luminescent properties manipulation via interaction with silver nanoparticles in aqueous solutions. J-aggregates are nanoclusters of non-covalently bounded organic dye molecules. They possess unique optical properties due to delocalization of electronic excitations that make them suitable as fluorescent probes for biomedical applications, organic light-emitting diodes, photoelectronic converters, etc. To control a distance between J-aggregates and nanoparticles the later has been coated with different number of polymer layers using L-b-L techniques modified for colloidal solutions. By varying an amount of polymer layers, we have achieved both quenching and increasing luminescence of the J-aggregates (Fig. 1).

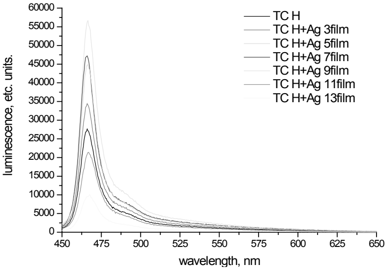

Fig. 1 The luminescence spectrum of J-aggregates with Ag nanoparticles in solution

ELLIPSOMETRIC STUDY OF NANOSTRUCTURED COMPOSITE MATERIALS

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Optical properties of $(Co_{41}Fe_{39}B_{20})_x$+$(SiO_2)_{100-x}$ composite nanostructure in amorphous state x = 100%, 56%, 41% and 33% were studied in this paper. The study of angular dependences of the samples' optical properties has been carried out in a range of angles of incidence $\varphi = 50 \div 80$, that includes the principal angle of incidence. A LG-56 He-Ne laser was used as radiation source ($\lambda = 632.8$ nm).

Based on the obtained data it was shown that the principal angle of the studied samples depends on the metal content of the composite. Calculated optical properties based on these data were found to depend strongly on the angle of incidence, which was attributed to the influence of the surface layer, removed afterwards by chemical etching. A 15% water solution of sulphuric acid was used for these samples. The ellipsometric parameters Δ and ψ measurements have shown that the optimal etching time for these composites was 7 seconds. In this case the dependences of optical properties, such as the refraction and absorption indices n and χ, dielectric permittivity ε and optical conductivity σ, on the incidence angle φ are described by smoother curves than the original samples. It indicates a notable improvement in composites' structure near the optical surface.

The study of the ellipsometric parameters' Δ and ψ dependences on the incidence angle φ for $(Co_{41}Fe_{39}B_{20})_x$+$(SiO_2)_{100-x}$ nanocomposite structures in amorphous state with different contents of the metallic component has revealed that such dependences are described by smooth curves for all samples. With the decrease in the metallic component content in the composite the principal angle of incidence increase.

EVOLUTION OF GOLD NANORODS OPTICAL ABSORPTION INDUCED BY FEMTOSECOND LASER IRRADIATION

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Metal nanorods attract a lot of attention due to tunable surface plasmon properties that could be used in chemical separation and sensing. Among the metals with prominent plasmonic properties in visible part of spectra, gold is often used because it is chemically inert and biocompartible. Interaction of femtosecond laser pulses with metal nanoparticle results in surface plasmon excitation and accompanying local field enhanced Kerr effect in surrounding media, followed by multistage relaxation: loss of the phase coherence of electrons, electron-phonon energy transfer, and lattice cooling.

The samples, colloidal solution of gold nanorods in water, prepared at University of Mainz, were characterized by optical absorption spectroscopy and dynamic light scattering. We studied changes of both longitudinal and transverse localized plasmon modes in gold nanorods upon irradiation by femtosecond laser pulses. Studies were performed by femtosecond pump-probe technique using fundamental radiation or second harmonic of Ti:Sapphire laser as a pump beam and "white light continuum" as a probe beam. Induced changes of optical absorption of the sample, namely, plasmon peak position, height and FWHM, were investigated with sub-picosecond temporal resolution. Besides reversible rapid changes of the optical properties, irreversible nanorods transformation (aspect ratio change) was observed. Pump-probe measurements were performed at Center for collective use Femtosecond Laser Complex of National Academy of Sciences of Ukraine.

MANIFESTATION OF THE α-QUARTZ PHASE IN RAMAN SPECTRA OF SYNTHETIC OPALS WITH MELTED-IN $Li_2B_4O_7$ DOPING

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As a prototype of 3D photonic crystals synthetic opals consisted of SiO_2 globules are widely used. Doping opals by different substances one can obtain regular nanostructures with unique optical properties.

This work is devoted to filling opal pores with $Li_2B_4O_7$ and to studying Raman spectrum of obtained samples.

The filling was carried out by melting-in fine dispersive polycrystalline $Li_2B_4O_7$ powder at temperature slightly above the melting temperature T_m = 917 ^{0}C during for 5 – 20 min. An evidence of the pores filling was a vanishing of the opal iridescence when being illuminated in a visible light. Raman spectra of initial and filled opals were measured by using laser spectrometer on the base of double monochromator DFS-12. X-ray study of initial opals was performed with the diffractometer DRON – 2.0.

Both X-ray diffraction and Raman spectra testified an amorphous state of initial opals. Raman spectra of the obtained samples were different from each other depending on their melting-in duration. For sample with a shorter melting-in duration the spectrum consisted of bands attributed to shifted bands in $Li_2B_4O_7$ crystal spectrum and an intensive band of α-quartz at 470 cm^{-1}. For samples with a longer melting-in duration Raman spectra were identical to the α-quartz spectrum placed on the background of wide bands corresponding to amorphous state of the SiO_2 globules.

The work was performed with financial support of the Ukrainian-Russian project "Creation and investigation of active matrix nanocomposites on the base of photonic glasses and crystals for solar cells".

FORMATION OF SUPRAMOLECULAR STRUCTURES OF N,N-DIMETHYLQUINACRIDONE IN BINARY SOLVENTS

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Quinacridone derivatives which are characterized by the formation of crystalline structures with intermolecular NH-O hydrogen bonding are perspective for use as elements of optoelectronic devices. Special case constitutes N,N-Dimethylquinacridone (DMQA), as far as the methyl groups on the nitrogen atoms prohibit the formation of intermolecular NH-O hydrogen bonding. It is assumed that the crystal structure and optical properties of DMQA is substantially different from those of quinacridones.

We carried out spectral studies of solutions of DMQA in DMSO when changing concentration within 0,1-0,0001 mg/ml. In the crystalline state DMQA has purple color, and when dissolved in DMSO it pass into the molecular shape and obtain yellow-orange coloring, which is consistent with the results of studies and quantum mechanical calculations for other quinacridone derivatives. Long-wave band of absorption has maximums at 460 nm, 490 nm, 525 nm, while band of luminescence has maximums at 545 nm, 575 nm. The intensity of the absorption and luminescence directly proportional to the concentration, indicating a lack of formation of supramolecular structures DMQA in single solvent DMSO.

On adding to the solutions DMQA in DMSO of traces (very small amounts) of other solvents, in which DMQA are insoluble, coloring of the solution into light purple color and changing of its spectral characteristics are observed. In the absorption spectrum appears an additional band with a maximum at 560 nm, and the luminescence spectra remain unchanged, though the intensity of luminescence decreases several times. Given that the maximum of absorption of crystalline DMQA is 580 nm, the obtained results testify formation of non-luminescent supramolecular structures of N,N-dimethylquinacridone in binary solvents. The nature of these structures requires further research.

INTERACTION BETWEEN POLYMETHINE DYE MOLECULES AND CdSe NANOPARTICLES IN AQUA SOLUTION

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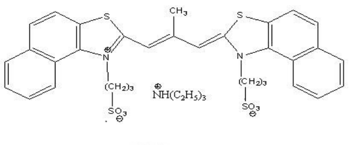
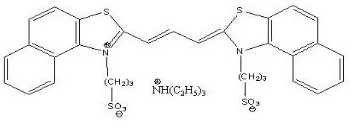
We present the results of studying the interaction between polymethine dye molecules and CdSe nanoparticles (NP) in aqua solution. Combination of these two objects in one light absorbing and emitting system is one of the actual tasks now. It can be possible to increase the luminescence of them by resonance energy transfer. Energy transfer is possible in both directions: from NP to J-aggregate and from dye molecules to NP. Separate scarcely studied problem is process of adsorption of dye molecules on NPs surface. Studying the influence of aggregation on the NP surface to the light absorption, excited stay decay and photo induced decay processes of dye molecules is also an important task.

We were studying the dye that can form aggregates in aqua solution (Dye1) and the dye, that don’t forms aggregates (Dye2). Nanoparticles of cadmium selenide were chosen because of the proximity of their absorption bands and absorption bands of Dye1. That allows to expect the formation of the system (NP+dye) molecules with resonance energy transfer. Additionally CdSe NPs are comfortable and well-studied objects with a wide area of possible practical applications.



Dye1



Dye2

For the both dyes was observed that the presence of the NPs leads to growing of the time of dye discoloration. One of the possible reasons for such dye stabilizing is the adsorption of dye molecules on NP’s surface. Apart from that was observed that process of aggregate forming starts at low concentrations (1×10^{-5}M) of dye1 in presence of NPs, without NPs forming of J-aggregates does not occur at that concentration. Possible reason for that is local increase of dye concentration around of the nanoparticle that caused with gradient of electromagnetic field around it. As a result, occurs interaction between NP and polar molecules of dye, that leads to formation of aggregates of dye molecules.

TEMPERATURE DEPENDENCE OF RAMAN SPECTRA OF SINGLE-WALLED CARBON NANOTUBES

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Since their discovery, carbon nanotubes (CNTs) have been predicted to be the most reliable components of the next generation electronics due to their extraordinary electrical properties. Moreover, thermal stability and temperature dependence behaviors are very important for such CNT-based devices. In this case, resonance Raman scattering should be a very effective and nondestructive tool for detecting nanotube's properties. Specially, the temperature dependent Raman spectra in CNTs can allow us to understand their fine structure information and properties, such as atomic bond structure, thermal expansion, specific heat, and thermal conductivity.

We have presented experimental results describing the temperature variation in the Raman spectra of SWCNTs nanotubes in temperature region 4 – 300 K.. We have analyzed fundamental and combinated modes frequencies shift as a function of temperature.

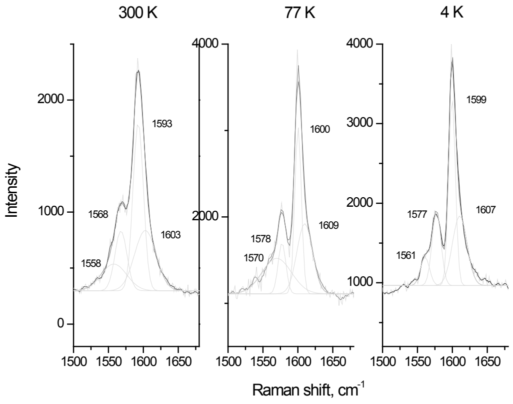

Fig.1. Raman spectra of G-mode of SWCNTs at temperature of 300, 77, and 4 K

7
SURFACE

EFFECT OF RESONANCE DIPOLE-DIPOLE INTERACTIONS ON SPECTRA OF ADSORBED SF_6 AND NF_3 MOLECULES

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Lateral interactions, studied in detail by IR spectroscopy for CO adsorbed on metals [1] and oxides [2], affect greatly the adsorption and catalytic properties of solid surfaces. The method of isotopic dilution enables us to distinguish two kinds of interactions: static effect and the dynamic interaction, referred also as resonance dipole-dipole (RDD) interaction or dipole coupling. The former affects the strength of surface sites and often determine the geometry of adsorbed layer, while the latter modifies the positions, shapes and widths of absorption bands in the spectra of adsorbed molecules. It accounts also for the vibrational energy exchange in the adsorbed layers and cannot be neglected when considering the dynamics of resonance excitation or the energy dissipation processes

Up to now, the RDD interaction has been observed only for CO molecules somehow oriented with respect to the flat surface of crystals. Recently it was shown, however, that complex band shapes in the spectra of such molecules as SF_6, CF_4 and NF_3 in liquid or dissolved state can be explained by RDD interaction [3]. The aim of this work was to find out the manifestations of such interactions in the spectra of SF_6 and NF_3 adsorbed on the surface of amorphous or crystalline oxide adsorbents.

To simulate the effect of RDD interaction upon the band shapes of adsorbed molecules we used the modified model developed in our previous study [3]. Three different variants of mutual arrangement of molecules were considered: i) three-dimensional system as in the case of solid film, ii) 2D structure of adsorbed layer on the flat surface, and iii) 1D chain- like structure that had to reproduce the filling of zeolite (silicalite) channels with the adsorbed molecules. The results obtained as shown are in quantitative agreement with the experimental data.

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EFFECT OF LASER IRRADIATION ON OPTICAL PROPERTIES OF CdS THIN FILMS FOR SOLAR CELLS

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Cadmium sulfide (CdS) is suitable as transparent semiconducting material for the fabrication of photovoltaic (PV) solar cells. The presence of impurity and defect centers, which acts as recombination centers for charge carriers, can reduce the PV conversion efficiency. The irradiation of pulsed Nd:YAG laser (wavelength λ=532 nm, pulse duration τ=4 ns) of different intensities was used for the improvement of the quality of CdS film formed by closed space sublimation (CSS) method on ITO/glass structure.

Low-temperature reflection and photoluminescence (PL), kinetics of the room-temperature PL have been studied. The energy position of free excitons obtained from reflection measurements allow to define unambiguously the structural type of obtained layer after the laser processing. The effect of the laser irradiation of studied films manifests itself in considerable change of Pl spectrum of irradiated CdS film as compared with non-irradiated film. Namely, after the irradiation the intensity of bands related to defect states (for example, vacancies or interstitials) at 1.78 eV and 2.2 eV decrease, while the sharp band at 2.55 eV attributed to the free exciton recombination becomes much more defined and intense. Analysis of the PL decay curves reveals the contribution of slow and fast decay components of PL and allows to estimate the decay times for nonradiative and radiative recombination processes in non-irradiated and irradiated CdS films. Observed changes of optical properties demonstrate that the CdS films undergo changes under laser irradiation, for example partial melting and following recrystallization of surface layer. Thus, irradiated CdS films demonstrate improved quality.

PECULIAR PROPERTIES OF ABSORPTION AND PHOTOLUMINESCENCE SPECTRA OF POROUS SILICON CARBIDE

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Porous silicon carbide (por-SiC) is attractive as a matrix for the nano-structured materials. The porous layer allows to obtain more perfect epitaxial layers in multilayer heterostructures (in particular, during deposition of GaN layers in the process of the LEDs manufacture).

The spectra of absorption and photoluminescence (PL) of por-SiC, obtained by anodic etching in hydroalcoholic solution of hydrofluoric acid: H_2O: HF: C_2H_5OH = 1:1:2, current density - 20 mA/cm^2, etching time - 5 min, have been studied.

Comparative analysis of PL spectra of por-SiC for different values of the excitation energy: $h\nu_{ex}$=3.67 eV ($h\nu_{ex} > E_g$ 6H-SiC), 3.05 eV ($h\nu_{ex} \approx E_g$ 6H-SiC) и 2.54 eV ($h\nu_{ex} < E_g$ 6H-SiC) demonstrates that at $h\nu_{ex} \leq E_g$ the PL band of 2.75 eV disappears, and the intensity of the band at 2.15 eV significantly increases. The band at 2.15 eV in PL spectrum is associated either with the appearance of fine cubic phase of SiC in porous layer, either with the impurity-surface states formed on the sample surface during the etching, and due to the residues of the chemical reactions products.

The presence of the cubic phase of SiC in porous layer can be identified from absorption spectra. Since the band gap of c-SiC (2.4 eV) is smaller than the band gap of 6H-SiC (3.02 eV), SiC cubic phase in por-SiC layer should manifest itself in the absorption edge shift. In our case, the formation of the porous layer on the surface of 6H-SiC crystalline substrate results in the increase of absorption throughout the spectral region under investigation, but the position of the absorption edge remains unchanged.

The obtained data allow to conclude that the PL of por-SiC at $h\nu_{ex} \leq E_g$ is due to the surface states caused by the impurity atoms, surface defects, complex compounds (such as oxides and siloxenes), or the saturation of Si-H or C-H bonds that arise, in particular, during the etching.

OPTICAL PROPERTIES OF Co-O STRUCTURES

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Optical properties of Co-O structures were investigated in wide spectral range 0,25-17,0 μm (0,07 – 4,96 eV) by Beattie spectroscopic ellipsometry method. During experiment ellipsometric parameters D and y were measured near principal angle of incidence and optical constants were calculated. There were established, that optical properties of metallic cobalt under structural changes “amorphous – crystalline states” determined by the nearest atoms and electronic structure did not change a lot. Based on the analysis of absorption curves for liquid, amorphous, crystalline FCC Co and HCP Co lattices was shown that calculated dispersion curves of optical conductivity only in general, describes experimental absorption spectra of amorphous and crystalline cobalt. After comparing experimental and calculated amorphous cobalt absorption spectra the formation of additional zone associated with vacancies and located at 0.38 eV below the Fermi level were established. The absorption spectra of Co-O systems (2 and 4% oxygen) in different structural states (amorphous and crystalline) than the main absorption bands characteristic of cobalt, the formation of new bands related to oxygen impurity. After analysis of the absorption spectra of Co-O (2% oxygen), in the amorphous state, defined position and half-width of the impurity band associated with oxygen. Also we calculate the density of electronic states within the impurity band, which formed approximately at 0.72 eV above the Fermi level in the subzone, which is formed by electrons with up-spin direct (↑).

EXCITATION SPECTRA OF THE Sb/Si(001) INTERFACES

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Electronic excitations play an important role in surface physics, because it can be used as promoters of some chemical reactions or photodesorption. So the investigation of excited states provides important information about the properties of adsorbed surface layers. Besides Si(001) surface structures, with submonolayer films of V group elements (As, Sb, Bi) could be used as a surfactants to improve heteroepitaxy Si/Ge. The aim of the work was in theoretical and experimental investigations of the excitation spectra of the Si(001) surface, covered with submonolayer Sb films.

Electronic excited states were studied using time–dependent density functional theory (TDDFT) in B3LYP/SBK++ and B3LYP/N31–6/SBK** approaching. The TDDFT absorption spectra of Sb/Si(001)–0.5ML and Sb/Si(001)–1ML surfaces were obtained. The position of the absorption maximum for Sb/Si(001) system is ~3.8eV in good agreement with experiment. The absorption maxima are identified with $\sigma(\text{Sb–Si}) \rightarrow \sigma^*(\text{Si–Si}_{\text{bulk}})$ transitions between bonding state of the Si–Sb backbonds and antibonding bulk states Si–Si.

The absorption edge for the Sb/Si(001)–0.5ML surface is formed by transition between silicon surface dimer bonding state and Sb–Sb addimer antibonding state. The absorption edge for the Sb/Si(001)–1ML surfaces is formed by transition between Sb–Si backbond bonding state and Sb–Sb addimer antibonding state. The absorption edge shifts towards higher energies with the antimony coverage increasing from 0.5 ML to 1 ML because of modification of the Si(001) surface structure.

Optical properties of Sb/Si(001) interfaces were investigated in a wide spectral range (1–4.5eV). Ellipsometric parameters ($\text{tg}\psi$ and $\cos\Delta$) were experimentally measured by the Beatty method, and spectra of the optical anisotropy were calculated. Experimental investigation of anisotropy demonstrated the ability to identify surface Sb/Si(001) interfaces by optical methods. It is shown that homogeneous Sb films may have some surface structure, which leads to optical anisotropy of the surface.

OPTICAL TRANSITIONS IN THIN Si FILMS

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Widespread silicon usage in solar energy causes need in detailed investigation of its structure effect on the optical transitions (optical transitions determine the electrical characteristics of Si solar cells). It is known that defects in crystal structure of silicon films significantly affect the efficiency of solar cells and, in general case, optical properties of the Si films depend, not only on the defects, but on their structure. This work is aimed at determining the optical properties of thin Si films from structure of defects in it.

Optical properties of the films were investigated in wide spectral range (250–1200nm) by the spectroscopic ellipsometry. Ellipsometric parameters (tgψ and cosΔ) were experimentally measured near the Si pseudo Brewster angle at different wavelengths, and spectra of the optical conductivity $\sigma(h\nu)$ were calculated. Optical studies have shown that the undoped nanocrystalline silicon films thickness increasing from 3 to 100nm leads to the shift of the absorption maximum at shorter wavelengths. In this case, there is a correlation between surface inhomogeneties size and the shift of the absorption maximum. The sharp increase of the relief inhomogeneties size of the Si films (if the thicknesses are more than 70nm) causes the additional absorption bands in the optical dependencies, which specify the type of film structure: fibrous or equiaxed.

STM INVESTIGATION OF THE Si(001)-8×8 SURFACE RECONSTRUCTION

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The ground state of atomically clean Si(001) surface in ultra-high vacuum is a well-known 2×1 ”dimer row” reconstruction [1]. However it’s relevance for practical applications is rather limited, as the actual conditions of technological processes in micro- and nano-electronic devices production are far from being impurity free and thermally equilibrium. These circumstances lead to Si(001) reconstructions of larger periodicities, such as: 2×n, 4×4 and 8×8 [2-3].

In this contribution we present the experimental results of the scanning tunnelling microscopy (STM) investigations of the Si(001)-8×8 reconstruction. The voltage dependent STM provides spectroscopic information on the distribution of electronic states in the valence and conduction bands. We have achieved atomic resolution in the empty states STM images and a dimer resolution in the occupied states. Analysing the dependence of atomic size features brightness on the bias voltage between the silicon sample and the STM probe tip, we have been able to assign these features to individual silicon atoms and suggest a novel structural model of the Si(001)-8×8, which is different from the ones found in the literature. Its basic building blocks are groups of three silicon dimers placed in a “brick wall” arrangement. Similar to the Si(001)-4×4 atomic structure, our suggested model is a “diluted” layer of silicon atoms (all at identical heights) with an areal density smaller than required to build a full Si(001) atomic plane.

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THREE-LAYER MODEL OF THIN METAL FILM USED FOR SPECTROELLIPSOMETRY INVESTIGATION WITH AND WITHOUT EXCITATION OF SURFACE POLARITONS

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A three-layer model of thin semitransparent metal film is proposed. The program of calculations of direct and inverse problem of spectroellipsometry using recurrence Airy formulas with and without excitation of surface polaritons was designed. Experimental study of ellipsometric parameters, namely the azimuth of a restored linear polarization Ψ and the phase shift Δ between the *p*- and *s*-components of reflected light using the method of Beatty for different wavelengths with and without excitation of surface polaritons for thin Ti and Mo films of varying thickness was conducted. Experimental studies and theoretical calculations showed the following. Solving the inverse problem for spectroellipsometry using experimentally measured ellipsometric parameters Ψ and Δ for 5 angles of incidence of light on the sample without excitation of surface polaritons has shown that the middle layer of the film in a three-layer model is corresponding metal. Its optical constants coincide with optical constants of corresponding bulk metal. The upper and lower layers are oxides of this metal. The obtained optical constants do not depend on the thickness of the film, which has practically no place in the conventional single-layer film model. Another pattern is observed during excitation of surface polaritons. The calculated and experimentally measured angular and spectral dependences of ellipsometric parameters coincide only qualitatively. The course of both curves in the figures is quite identical. Quantitative coincidence is poor. The latter can be explained as follows. In the considered three-layer model the boundaries between layers were assumed ideally planar. At the same time, the real boundaries are rough and inhomogeneous. For specroellipsometric studies without excitation of surface polaritons latter feels less, because of wavelength of the light which is much larger than the film thickness so it is larger then the value of surface irregularities. The surface polaritons risen in experiments feel irregularities and inhomogeneities of the surface quite strongly, while propagating along it. The latter leads to a disagreement between theoretical and experimental results in the case for excitation of surface polaritons.

APPLICATION OF ISOTOPIC SUBSTITUTION IN THE FTIR STUDIES OF SYSTEMS WITH LINKAGE ISOMERISM

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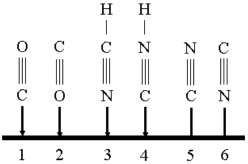
Adsorbed complexes with linkage isomerism, first established for CO molecules adsorbed on cationic forms of ZSM-5 and Y zeolites [1], could be important for establishing the mechanism of catalytic reactions. In fact, thermally activated energetically less favorable isomeric forms, such as CO molecules bound to the cations via oxygen atom, have the excess of energy, as compared with usual C-bonded species, and can be considered as the activated intermediate state in the reactions of carbon monoxide with other molecules [2]. However, the assignment of the two bands, shifted to the opposite directions with respect to the frequency of gaseous CO was based mostly on the intensity measurements as a function of temperature. In this work we applied isotopic substitution to establish the structure of adsorption complexes with linkage isomerism. For CO adsorbed on ZnY, ZnZSM-5 and CaY zeolites, as well as on γ-Al_2O_3 the bands assigned to C-bonded species (structure 1 in scheme 2) exhibit the shift caused by ^{13}C substitution 1.0-1.8 cm^{-1} greater than that following from the reduced mass ratio. For the low-frequency band of O- bonded CO (structure 2) in the spectrum of CaY zeolite, on the contrary, it is 0.6-1.5 cm^{-1} less. HCN interaction with oxides and zeolites could lead to different isomeric species both for molecular (structures 3,4) and dissociative (structures 5,6) adsorption [3]. Then, admitting of deuterated compound enables us to distinguish between the bands of molecules and CN^- ions, while the choice between the isomeric structures 3 and 4 or 5 and 6 can be done using the results of ^{13}C and ^{15}N substitution. Such data show that HCN dissociation on γ-Al_2O_3 leads first to the formation of Al-NC species with isotopic shifts differing by up to 5 cm^{-1} from those calculated from the reduced mass of the C-N group, in agreement with the assignment proposed by Yates et al [4].



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THICKNESS DEPENDENCE OF REFRACTIVITY IN WALL-ADJACENT ELC LAYERS

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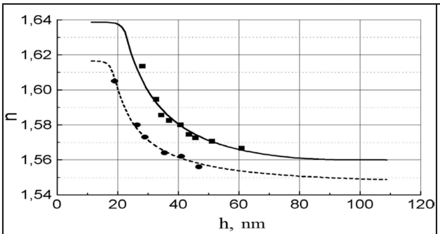
Under certain conditions a solid substrate may induce an orientational ordering in wall-adjacent layers (so called epitropic liquid crystals – ELC). Optical properties of these layers were studied experimentally by different methods. The results of ellipsometrical investigation of nitrobenzene wetting films [1] were recalculated in the framework of Drude equation in order to obtain *n*(*d*) dependence. Polarimetric studying of plane light-guide [1] filled with studied liquid allowed us to determine the induced optical birefringence in symmetrically bounded interlayers, It was found that refractive index of the film sufficiently differ from the bulk one and that induced birefringence decreases vs layer thickness.. In order to explain this difference we used well-known Mayer-Saupe-Neugebauer model.

According to this model it is assumed that the mean value of molecular polarizability does not depend on the phase state of studied liquid and on its degree of orientational ordering. We determined that thickness dependence of mean value of refractive index may be written in the form $n(d) = \sqrt{a + b \cdot S(d)}$ Here *a* and *b* are fitting constants and $S(d)$ dependence was calculated earlier [2].



.Fig. 1. Thickness dependence of nitrobenzene wetting film refractive index– ■ – t =20 ⁰C, ● – t =50 ⁰C.

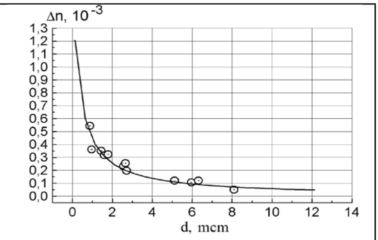


Fig.2. Thickness dependence of nitrobenzene symmetrically bounded interlayer birefrringence Δn(d)..

Experimental results and theoretical calculation (solid lines). Quartz substrate

Fig.1 shows that refractive index monotonously decreases vs the distance to the surface substrate and asymptotically approaches to the isotropic bulk value. Fig 2. illustrates that order parameter of the interlayer S is in fact proportional to its integral birefringence $\Delta n = n_{\Uparrow} - n_{\perp}$. $\Delta n(d) = a_1 S$

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GONIOPHOTOMETRY OF OPTICAL MEDIA USING PRECISION OBJECTIVE FUNCTION MINIMIZATION METHOD

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Angular and azimuth polarization dependences of photometric variables of light scattered by sample with concrete dielectric function may serve as an informative source on optical properties and features of intrinsic structure of such sample.

In order to determine these variables the automated goniophotometric installation on a base of a standard goniometer Г-5 is fulfilled. As a light source the semiconductor laser that emits at a wavelength λ = 655nm and possesses the power of 3 mW is used. The instrument permits to carry out the polarization measurements and obtain the polar dependences of the intensity of the scattered light as well as to determine dielectric function for optical media with different type of conductivity.

The method for determination of such optical characteristics as absorption coefficient and refractive index is developed. Optical characteristics of strongly scattered glasses and some standard filters (color glass) produced in Izum Optical Instrumental Plant, Kharkiv region, Ukraine, were measured.

To determine the optical constant of such glass samples the method involving measurement of a transmittance of sample within angles of incidence from 0 ° to 55 ° and using experimental results as preliminary ones for further approximation as well as a selection of the optimality criterion with its minimalization due to the precision objective function. Minimization of this function leads to obtaining the required characteristics. For laser radiation at a wavelength of 655 nm the absorption coefficients of several glass samples were determined. The accuracy of the numerical results of the absorption coefficient is of 0.5-1%.

The second important characteristic of the above-mentioned material within the visible is the refractive index. The method for obtaining this characteristic based on the Brewster's angle definition measurement is realized. Its mathematical algorithm may minimize the difference between the experimental and the calculated data using at least five experimental points due to different angles of light incidence. When the Brewster's angle is determined then it is possible to find the refraction index. The accuracy of its determination is of 1-3%.

In the installation the additional device using polarized light permits to provide the measurement of the Stokes parameters for scattered radiation and obtain the Mueller matrix of appropriate optical media at different angles of light incidence.

ELLIPSOMETRY OF CONTACT SURFACES AFTER THEIR TREATMENT BY FEMTOSECOND LASER PULSES

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We present ellipsometric measurements of the bonded area between optical materials joined according to the method from ref [1]. Assemblies that were inspected include fused silica-silica (sample 1), fused silica-copper (sample 2) and fused silica-silicon (sample 3). The bonded interface of each sample is composed of numerous laser weld seams at their periphery in a closed shape pattern so as to seal the inner part inside which optical contact is maintained. A Coherent REGA 9050 Titanium-sapphire femtosecond laser system with wavelength 790 nm and pulse width $\tau = 70$ ps was used for laser welding of the samples. The optical polarization parameters of the examined sample were evaluated using a laser ellipsometer with light wavelength $\lambda = 632$ nm. The ellipsometric parameters, such as the phase shift Δ between the p- and s-components of the polarization vector and the azimuth Ψ of the restored linear polarization, were obtained as dependencies on the light incidence angle φ. The azimuth of samples 1 and 2 did not demonstrate any feature in comparison to the typical curve $\Psi(\varphi)$ attributed to the dielectric media. Therefore, conclusive measurements of $\Delta(\varphi)$ and $\Psi(\varphi)$ were not obtained for the 3 samples. The angular dependencies $\Delta(\varphi)$ of the fused silica-silica sample are plotted in Fig.1 for a range of angular values including the Brewster's angle φ_B as defined at $\Delta = 90°$.

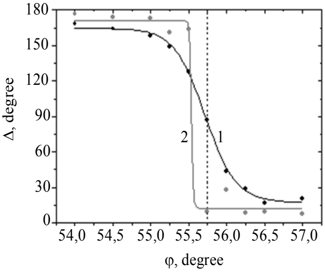

Fig.1. Angular dependence of the ellipsometric parameters Δ for the central area (optical transmission window) (curve 1) and the weld seam (curve 2) of the fused silica-silica sample

The value of φ_B for the weld seam is slightly less than the value φ_B of optical transmission window. The dependence $\Delta(\varphi)$ for optical transmission window of the fused silica-silica sample is characterized by smoother curve. However, there is an abrupt change of ellipsometric parameter Δ in the vicinity of the Brewster's angle for the weld seam of the fused silica-silica sample. Such behavior of ellipsometric parameter Δ may be explained by the material modification inside glass following femtosecond laser irradiation. This change is typically characterized by a densification and change in refractive index, and may also be characterized by a strong birefringence inside the welded area.

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STRUCTURIZATION OF UNSATURATED HYDROCARBONS NEAR METALLIC SURFACES

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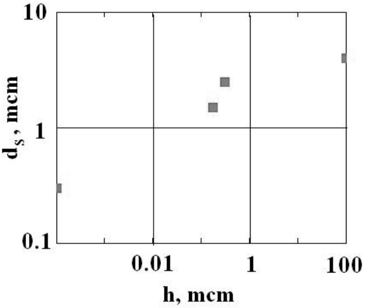
We studied the peculiarities of structure of orientationally ordered wall adjacent layers of some nonpolar organic liquids with long chained molecules (epitropic liquid crystals – ELC) near solid substrates of different nature. It was measured the dichroism of admixtured absorption of dilute sudan solution in unsaturated hydrocarbon hexadecane $(C_{16}H_{34})$, which is characterized by high degree of molecular anisometry. The method allowed us to obtain the reliable results under the condition of isomorphism of guest and host molecules.

Earlier [1-3] it was found the anomalous behavior of IR, UV absorption spectra and reological characteristics of thin interlayers of this liquid, which is connected with formation of ELC layers with homeotropic texture near solid substrate.

We used two different geometries of our experimental cell – "on the lumen" (liquid in the layer) and "along the layer" (liquid in the gap). In the first case quartz substrates were covered by ultrathin semitransparent metal film and in the second one– the specimen was placed between two non-transparent metal plates.



It was found that the nature of the substrate essentially determines the ELC thickness in contrary to the value of the order parameter S of the layer which is almost the same (S~0.27-0.33). Fig.1 illustrates the dependence of ELC layer thickness d_s vs the thickness h of metal film disposed on the substrate.

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WETTABILITY AND MORPHOLOGY PROPERTIES OF POLYTETRAFLUOROETHYLENE TREATED BY γ-IRRADIATION NEAR THE MELTING POINT

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Polytetrafluoroethylene (PTFE) has gradually developed to become the material in numerous applications. By virtue of its versatile characteristics, its potential use in a modern technological society appears limitless— ranging from electrical and electronics, biomedical, mechanical and chemical to agricultural and aeronautical applications. Among the disadvantages of PTFE are high creep coefficient, low wear resistance and low radiation resistance. γ-irradiation of PTFE at temperature above the polymer melting point is a promising technique which imparts unique properties to PTFE. But the nature and the structure of PTFE modified in this way are still not enough understood. Earlier we have shown that PTFE subjected to γ-irradiation under this condition gains color and fluorescent properties [1,2].

In the present work wettability and optical transmittance properties of γ-irradiation of PTFE were evaluated using contact angle, scanning electron microscopy tests. Irradiation below the melting point does not change quantitatively PTFE morphology. PTFE structure rearranges drastically under irradiation above the melting point. New morphology units, spherulites of size about 50 mm, are formed, the spherulites consisting of radially extending fibrils, and porosity decreases substantially. The change in surface energy with irradiation treatment was assessed by measurement of the sessile contact angles. It was evident that an increasing irradiation dose did not result in an appreciable change of wettability. Samples of PTFE irradiated in air exhibit greater hydrophilicity and less transparent than the irradiated samples in vacuo at a temperature of melting.

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LASER-INDUCED INCANDESCENCE OF SURFACE LAYERS WITH TEMPERATURE-SENSITIVE ABSORPTION COEFFICIENT

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As is known, powerful pulsed laser irradiation of light-absorbing objects (microparticles, surfaces) produces visible thermal emission (laser-induced incandescence, LII). Such pulsed thermal emission is observed in soot aerosols, organic fuel combustion flames, suspensions of black particles, polymers and oxide glasses with particulate impurities, surface layers of materials with high enough absorption coefficients, etc. A distinctive feature of LII is its essential non-linear response to the variations of laser excitation power. The non-linearity of LII seems to be a promising property for possible applications for monitoring the processes under powerful laser irradiation. For example, the factor of non-linearity of single-wavelength LII can be used for estimation of temperature of laser-heated objects.

In the present work we investigate theoretically the effect of temperature-induced changes of absorption coefficient of laser-irradiated surface on the non-linear properties of LII. Calculations of local temperature values inside the sample were performed with the use of heat transfer equation

$$\mathrm{div}\left(\kappa\ \mathrm{grad}T\right)+W=c_p\frac{\partial T}{\partial t}$$

with pulsed-laser heat source function $W\left(\vec{r},t\right)=\alpha F\left(\vec{r},t\right)$

for a bell-shaped laser pulse with duration of 20 ns and Gaussian cross-beam laser power distribution. The values of pulsed LII signals I_{LII} were calculated with the use of Planck's blackbody function by integrating over the irradiated surface and over time.

In the calculations, the dependence of absorption coefficient on temperature was considered as linear and non-linear growth. The results of calculations show that the increase of absorption with temperature causes significant effect on the behavior of LII with changing the laser power. For temperature-sensitive surfaces, the non-linearity factor $\gamma=\left(\mathrm{d}I_{\mathrm{LII}}/I_{\mathrm{LII}}\right)/\left(\mathrm{d}F/F\right)$ becomes a rising function of laser power F, whereas usually for $\alpha=const$ factor γ decreases with the increase of F. The effect is most pronounced for non-linear functions $\alpha\left(T\right)$. The possibilities of experimental observation of the predicted effect are discussed.

LASER-INDUCED INCANDESCENCE OF SILICON UNDER 1064 NM EXCITATION

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When laser radiation heats up the absorbing media skin layers to incandescent temperature, the observed thermal emission is called LII (laser-induced incandescence). It is supposed that LII can provide useful information for laser surface treatment, monitoring of surface temperature, roughness, presence of protective layers on the surface etc.

In this work we studied the LII of a crystal silicon surface under YAG:Nd laser irradiation. Lasing wavelength in this case corresponds to the fundamental absorption edge which results in low absorption and in a possibility to heat up a relatively thick surface layer of the sample. Also due to a strong temperature dependence of absorption coefficients of silicon there is a possibility to realize a nonlinear absorption LII experiments.

The experiments show that incandescence of silicon surface in the visible spectral range appears after a preliminary surface irradiation by a few tens of laser pulses with the intensity above the threshold (approximately 150 MW/cm2). Besides, the appearance of LII was accompanied by appreciable changes of physical characteristics of the irradiated spots, including the surface morphology which was investigated with the use of AFM. Possible mechanisms of the observed increase of LII with the irradiation dose are discussed.

For a laser-irradiated spot of silicon surface, it is observed that the parameter of non-linearity of LII

$$\gamma = \frac{\mathrm{d}I_{\mathrm{LII}}/I_{\mathrm{LII}}}{\mathrm{d}F/F}$$

increases with the increase of laser excitation power F. Such behavior seems to be anomalous as compared with other objects (carbon black suspensions, carbon surfaces, carbon-doped glass). As a mechanism of the mentioned abnormality the dependence of absorption coefficient on temperature is considered.

8

BIOMOLECULES AND POLYMERS

RAMAN SCATTERING OF DNA IN CONFINED VOLUME OF PHOTONIC CRYSTAL

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Active search for new materials with controllable optical properties has resulted in the invention of new class of optical materials called photonic crystals. These materials consist of periodically arranged dielectric globules or cavities with sizes comparable to the wavelength of light [1].

An infiltration of biological molecules in PC leads to a change of dielectric property of environmental medium between the structural elements of PC and the change in stop zone formation. On the other hand, the optical property of biological molecules, introduced in the confined volume of the photonic crystal air holes, could be changed also. DNA, being a unique molecule, has a size that is close to the spacing between structural elements in synthetic opal. That is why the goal of our study is to register Raman scattering (RS) modes of separated DNA molecules in confined volume.

In our experiments we used the DNA water solution (1 mg/ml). RS spectra have been registered with Renishaw in Via Raman microscopy instrument in the 200-2000 cm^{-1}. Nanodisperse silica globules were synthesized by the Stöber method[2]. Growth of the photonic crystals was achieved by subsequent natural sedimentation.

The RS marker bands of DNA were drastically changed after its infiltration in the porous of opal. A structure of the DNA molecule in confined volume could be used as a model of DNA folding in the living cell.

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INTERMOLECULAR INTERACTIONS IN A TERNARY SYSTEM “GLYCEROL – PHOSPHOLIPID – WATER”

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An important aspect of modern biophysical studies concerns interaction of biologically-active substances with model lipid membranes. Alongside with drugs and vitamins the same approach seemed also promising for cryoprotectors, e.g. glycerol and its derivatives.

The ternary system “glycerol – dipalmitoylphosphatidylcholine (DPPC) – water” has been studied by differential scanning calorimetry (DSC) in a wide range of glycerol to lipid ratio (GLR) values. Shifts of the DSC peaks of phase transitions of the DPPC-based multibilayer structure (ΔT_m and ΔT_p – the main transition and pre-transition, respectively) were plotted as function of GLR (the method of quazi-binary phase diagrams). The obtained dependences appeared to be non-monotonous and sign-changed. The largest positive ΔT_m corresponded to GLR ~5, and the change in ΔT_m sign was observed at GLR ~ 7. When plotting ΔT_m and ΔT_p against glycerol concentration in water, the character of the dependence remains unchanged (the corresponding glycerol concentrations are ~45 and ~60 wt. %).

The result obtained points on the complex character of intermolecular interactions in the system. FTIR spectra have been obtained, confirming the presence of specific interactions between the system components. Implications of the obtained results for further understanding of cryoprotector properties of glycerol are discussed.

THE SPECTRAL RESPONSE OF THE INTERACTION BETWEEN OLIGOADENYLATES AND HIGH-MOLECULAR PROTEINS

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The biological macromolecules of the ribonucleic acids (DNA and RNA) and high-molecular pi-electron-containing proteins are well known as vitally important high-molecular compounds for all living organisms. They are the smallest building blocks of any living creature that is why interactions between them play a significant role in the functioning of all biological systems. Furthermore, synthetic nucleotide derivates ("small" molecules comparing with the biomacromolecules mentioned above) that can bind to a specific target macromolecule are used in the medicine as immuno-modulators and antivirus drugs. The electronic properties of all these compounds are connected with presence of the chromophores (pi-electronic groups) in their cells and manifested in the optical (near "biologically active" ultraviolet, visual and near infrared) wavelength range. Thus, these properties and any changes of them induced by chemical or conformational changes can be detected using optics spectroscopy.

The electronic energy structure of the ribonucleic acids and high-molecular proteins were the main objects of many researchers and studied enough (see, for example, our work [1]). But mechanisms of the interaction between these biomacromolecules are not clear for possibility to control the processes of this interaction and to produce new effective drugs. This work is devoted to the study of these mechanisms. The optical absorption, fluorescence and phosphorescence of the monomers (nucleotide: adenine (A), amino acids: tripthophane (Tr), Tyrosine (Ty), phenilalanine (Ph)), "small" synthetic nucleotide derivates containing A-links (oligoadenilates), binary solutions of the DNA / RNA / oligoadenilates with high-molecular pi-electron-containing proteins, the mixtures of A with Tr / Ty / Ph were investigated. The mixtures were prepared under specific conditions. The spectral response of the binding of the oligoadenilate to the proteins was fixed: the complexes (like AT-complexes in the DNA) between A and amino acids are formed. The mechanism of these complex formations is studied and discussed.

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STUDY OF THE SELF-ASSOCIATION OF DNA-BINDING DRUGS USING DOSY NMR SPECTROSCOPY

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In the present work we used Diffusion Ordered NMR SpectroscopY (DOSY, 600 MHz) to determine thermodynamic parameters of the self-association of the set of typical drug molecules which bind with DNA by intercalation or minor groove binding modes. The set of self-association models, either dependent or not on the hydrodynamic shape of aggregates, have been applied in order to evaluate the values of the equilibrium association constant, *K*, viz. dimer, indefinite association (EK-model), cylinder, ellipsoid and sphere, each of which includes or excludes the intrinsic attenuation of the association constant on aggregate growth. As a reference we used *K* values of constants derived from a ^{1}H chemical shift dataset using the EK model, the most widely used approach to study molecular assembly by means of NMR. The results of computations over a large set of molecules have shown that none of the tested models was able to reproduce the *K* values derived from chemical shift measurements for the whole series of studied molecules. An alternative approach based on the empirical dependence of diffusion coefficient of an aggregate as a function of the number of molecules in it was suggested and showed the most satisfactory agreement with ^{1}H chemical shift data. These results open up the possibility of further application of DOSY NMR to study molecular hetero-association in solution.

THE Co AND Ni IONS EFFECT ON THE DNA MACROMOLECULE SPECTRAL PROPERTIES AND PHOTOSTABILITY

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Specificity of biological reaction (metal – deoxyribonucleic acid(DNA)) allows, for the low concentrations of heavy metals, define and estimate influence of these metals on the DNA macromolecule and to the DNA degradation rate. The purpose of this work is research the influence of metal ions on the spectral properties of DNA.

The studies of the physical aspects of interaction of Co and Ni ions with DNA are useful for understanding the low-level mechanism of their interaction. Optical methods of investigation have significant advantages over other methods because they are non-destructive and can be used to study investigated materials in different states.

The optical absorption, fluorescence, phosphorescence in UV and visible spectral range, and effect of light irradiation on spectral properties of DNA with presence of cobalt and nickel ions are studied. Quantity of metal ions varies from 1 ion to 500 base pairs of DNA to 2 ions per one base pair.

It is shown that the shape of fluorescence and phosphorescence spectra of the DNA do not change in presence of cobalt/nickel ions, but their intensity depends on number of metal. Influence of Co and Ni ions on the DNA luminescence is compared. The possible mechanisms of interaction and excitation transfer ways were examined.

The conclusions concerning the influence of cobalt and nickel ions of different quantity on the DNA photostability were made.

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APPLICATION OF THE MAXIMUM ENTROPY METHOD TO THE ACOUSTIC SPECTRA ANALYSIS IN PROTEIN SOLUTIONS

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Acoustic spectra of protein solutions comprise rich information on the internal dynamics of solvated globule in the entire sub-nanosecond to microsecond range. To extract this information investigators usually apply the least squares fit of the measured sound attenuation spectra to theoretical expression denoting a sum of a preassigned number of discrete relaxation terms. Such simple approach, in favorable cases, allows of retrieving kinetics of thermally driven transitions between protein conformational states. However, due to multiplicity of protein conformational states, the choice of the number of relaxation components is often complicated leading to ambiguity of the analysis results [1, 2]. The most justified way of a multicomponent spectral decomposition, which yields a unique solution, is based on a maximum entropy method (MEM). MEM has been already used successfully in a variety of fields, including radio astronomy, NMR, fluorescence, and ligand rebinding.

In the present paper the MEM-assisted analysis has been first applied in acoustic spectroscopy. The sound attenuation spectrum of HSA solution measured in the previous study [2] has been decomposed into six discrete relaxation components by the adapted MEM algorithm. The relaxation times of four components observed on nanosecond scale have been assigned to conformational changes of the atomic groups located on the protein surface. Two additional kinetic components exhibiting microsecond kinetics have been considered to reflect mobility of rigid protein segments located in the globule interior.

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SPECTROSCOPY AND SIMULATION OF THE ELECTROACTIVE HYBRID POLYMERS CONTAINING IONIC LIQUIDS

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The development, investigation and implementation of electrolyte systems of different nature, notably organic liquid electrolytes, ionic liquids, polymer electrolytes and inorganic solid electrolytes, are of interest. In brief the electrolyte systems can be conditionally divided as follows:

- polymer + organic liquid (polymer gel)
- polymer + ionic liquid
- polymer + inorganic solid electrolyte + ionic liquids
- polymer electrolyte + ionic liquid
- polymer electrolyte + ionic liquid + liquid organic electrolyte
- ionic liquids + liquid organic electrolyte
- polymer electrolyte + inorganic solid electrolyte.

The blends consisting of two and more electrolytes are used and studied for obtaining electroactive polymer materials (EPM) with combined merits of selected electrolytes.

The present work shows (results of various structural studies) that the doping of the hybrid organic-inorganic polymer systems (HOIS) based on urethane oligomers (UO) and metal silicate (MS) by the molecules of ionic liquids (IL) based on morpholine leads to destruction of the mineral phase with the simultaneous formation of new crystalline structures due to MS/IL reactions. Contrariwise, synthesis of EPM based on UO and IL results in amorphous grain-oriented structural organization and formation of the ion conducting cluster with the DC conductivity level $\sigma_{DC} \sim 10^{-3}$-10^{-4} S/cm, AC conductivity level $\sigma' \sim 10^{-2}$-10^{-3} S/cm and permittivity $\varepsilon' \sim 10^{5}$-10^{6} (results of various spectroscopic studies).

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DEFINITION THE TRUE PHONON DISPERSION AND DETECTION OF THREE AMORPHOUS PHASES OF POLYETHYLENE

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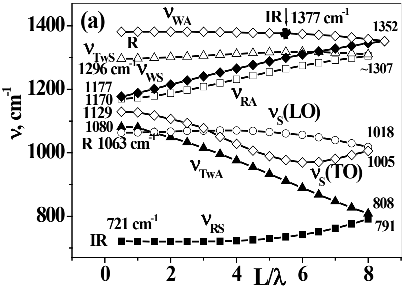
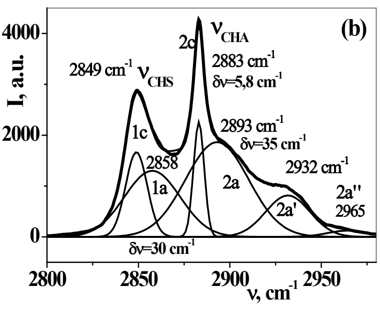
Regarding the phonon dispersion polymers ω(k), and in particular polyethylene (PE), in the literature there are large differences [1-4 etc.]. This is due to the arbit-rary choice force fields in the classical methods of calculating ω(k), and with the inaccuracies of quantum-chemical calculations (QChC). Even with QChC errone-ous results for the frequencies of transverse (TA) and longitudinal (LA) acoustic modes: $\nu_{TA} \approx 830$ cm^{-1}> ν_{LA} [2]. In this regard, we have carried out QChC (Gaus-sian-03), and detailed studies of the Raman (488 nm) and IR spectra of PE. Only a detailed analysis of the QChC and their coordination with the spectral data for the first time allowed us to find the true phonon dispersion of all 18 branches ω(k), part of which is shown in $C_{33}H_{68}$ for fig.a. Here L and **λ** - length PE molecule and the length of the vibrational waves, additional index S and A correspond to symmetric and antisymmetric vibration versatile CH_2 groups.

In many works is that the rocking $\boldsymbol{\nu}_R$, the twisting $\boldsymbol{\nu}_{Tw}$, wagging $\boldsymbol{\nu}_W$, defor-ma-tion $\boldsymbol{\nu}_\delta$ and stretching vibrations $\boldsymbol{\nu}_{CH}$ of the CH_2 groups PE form a separate zone. But from fig.a shows that vibrations $\boldsymbol{\nu}_{RS}$ coexist with $\boldsymbol{\nu}_{TwA}$, and $\boldsymbol{\nu}_{RA}$ - with $\boldsymbol{\nu}_{TwS}$ and just wagging vibrations $\boldsymbol{\nu}_{WS}$ and $\boldsymbol{\nu}_{WA}$ form a single phonon zone. On fig.b shows the structure of the valence band PE $\boldsymbol{\nu}_{CH}$ in the Raman spect-rum.





Together with the narrow lines nanocrystallites (NC) ~10 nm $\boldsymbol{\nu}_{CHS}$=2849 and $\boldsymbol{\nu}_{CHA}$=3883 cm^{-1} (1c, 2c) observation the wide bands 2858 and 2893 cm^{-1} (1a, 2a) of vibration $\boldsymbol{\nu}_{CHS}$ **and** $\boldsymbol{\nu}_{CHA}$ in the amorphous phase (AP). Two additional bands 2a' and 2a'' with frequen-cies of 2932, 2965 cm^{-1} and the observation of similar bands in the IR spectrum of the overtone $2\nu_{CH}$ convincingly demonstrated the presence of three AP of PE.

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COMPARATIVE STUDY OF SPECTRAL PROPERTIES OF dsDNA AND dsRNA VIRUSES

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Viral diseases belong to the most serious threats for the mankind nowadays. All virus particles (known as virions) contain the core with the nucleic acid (either DNA or RNA) that carry genetic information of the specific virus.

Mosquito iridescent virus *Aedes flavescens* (AfIV) is a large (200 nm in diameter) icosahedral lipid-containing virus which affects mosquitos of *Aedes, Culex, Culizeta* genera as well as freshwater fish and, therefore, can cause huge losses for industrial fish breedings. The AfIV virion consists of a core of genetic material (double-stranded viral DNA (dsDNA)), 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, especially trout and salmon. The IPNS virion consists of a double-stranded viral RNA (dsRNA)), surrounded by a protein capsid.

The aim of the work was to compare spectral properties of the AfIV and IPNV virions and 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 an efficient tool for distinguishing viruses of different type by means of optical spectroscopy.

Measured are absorption, fluorescence, fluorescence excitation, phosphorescence and phosphorescence excitation spectra of the AfIV and IPNV virions in different buffers at the room and low temperatures.

It is concluded that the analysis of low-temperature virion phosphorescence makes it possible to identify the type of nucleic acid (DNA or RNA) inside the virus.

THE PECULIARITIES OF THE DNA PHOSPHORESCENCE

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It is well known the biological macromolecules of the ribonucleic acids, DNA and RNA, are vitally important high-molecular compounds for all living organisms. On the one hand, they contain and transfer the genetic information, and together with high-molecular proteins are the smallest building blocks of any living creature. On the other hand, the electronic properties of these biomacromolecules are connected with presence of the chromophores (pi-electronic groups) in the nucleotide cells in their chains and manifested in the optical (near "biologically active" ultraviolet, visual and near infrared) wavelength range. This fact gives the ground to apply optics spectroscopy for the RNA / DNA electronic structure study. Finally, taking into account scientific works in biological engineering and the rising possibilities to modify the genetic information, the study of electronic properties of the DNA (including nature of phosphorescent centers) and interaction between its structural units are an important task of various areas of the science.

The electronic properties of the DNA / RNA were the main objects of many researchers (see, for example, [1]). But the majority of them did not clear the nature of luminescent centers of the RNA and DNA completely. The results of our previous works [2] showed the main triplet electronic excitations traps (responsible for phosphorescence) in the DNA, d(CCCGGGTTTAAA) oligonucleotide and a number of low-molecular nucleotide compounds are the complex formed by adenine (A) and thymine (T) chromophores. This work is devoted to the study of this complex nature. The optical absorption, fluorescence and phosphorescence of A and T monomers, their mixtures and the DNA were investigated. The mixtures were prepared under specific conditions. AT-complex in the mixtures is formed. The mechanism of this complex formation is discussed.

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THE SPECTRAL RESPONSE OF NEW HIGH-EFFECTIVE SENSOR ON THE PHENOL MOLECULES PRESENCE IN POLLUTED WATER

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One of the main tasks (connected with ecological problems) of the modern scientific world is the purification of natural water polluted by hazardous compounds. It is known there are some high-water-soluble compounds low concentrations of molecules of which even are very toxic. That is why the development of new high-effective principles, methods and equipments of such molecules detection and extraction from water is the very actual task. One of such compounds is phenol. On the one hand, the electronic properties of phenol are connected with presence of the chromophores (pi-electronic groups) in it molecules and manifested in the optical (near "biologically active" ultraviolet, visual and near infrared) wavelength range that can be detected using optics spectroscopy. In the present work the applying of optical spectroscopy methods to phenol express detection were examined.

On the other hand, the detection of extremely low concentration of phenol molecules requires the methods of some phenol molecules previous accumulation. The variant of this task solution is the use of functional polymer macromolecular complexes with spectral response (in optical range) and chemical structure that allows the non-native impurities to be sorbed from environment and easily detected by optical spectroscopy methods. For this purpose the intramolecular polymer complex – poly(vinylalcohol) with poly(acrylamide) grafted copolymer (PVA-PAA$_N$) – possessing such properties was used. In this work the investigations results of PVA-PAA$_N$ sorption properties by the optical spectroscopy methods were described, the mechanisms of phenol molecules sorption were discussed, and efficiency of purification of natural water by PVA-PAA$_N$-films was examined. The data obtained give the possibility to create the high sensitive sensors with the spectral response for the detection (and concentration measurements) of phenol molecules from polluted water. Besides, PVA-PAA$_N$ copolymer can be used for effective purification of natural water polluted by some hazardous compounds.

THE LUMINESCENT MATERIALS FOR POWER SAVING LIGHT SOURCES BASED ON CARBAZOLECONTAINING COMPOUNDS

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The electrical energy saving is an important problem for the conservation of natural resources. The significant part of produced energy is utilized by light sources. That is why one the main tasks of the modern technology world is the design of high efficient materials for effective energy saving source of light.

Our paper presents some results of investigations of the optical absorption and luminescence properties of vinilaromatic carbazolecontaining compound (specially designed for electroluminescent devices production) are presented. The effect of various technology film deposition on their spectra and intensities of luminescence were discussed. The compounds investigated are mainly chemical dimers, trimers of carbazole, two of them include five-six carbazole groups. The optical absorption, fluorescence and phosphorescence of these compounds in solutions, powders and films (obtained by two technologies of deposition) were studied at 293K and 77K. It is proved that the spectral properties of above mentioned compound in solutions are determined mainly by π-electron systems of carbazole groups and the weak interaction between them exists. The nature of luminescence (fluorescence and phosphorescence) 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 (with carbazole nature). In a number of cases the influence π-electron groups each other leads to domination the phosphorescence in luminescence spectra. The effects of difference in deposition technology on spectral properties of investigated compounds as well as their applications in sensor systems and OLEDs are discussed.

INVESTIGATION OF pH-DEPENDENCE OF THE OPTICAL PROPERTIES OF MELANIN IN AQUEOUS SOLUTIONS

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Melanins are perspective for physical studies due to their special characteristic - these polymers are electrical conductors showing photoconductivity in the solid state. However, this property appears only while humectation of melanin. In this regard, we studied of optical properties of melanin of natural origin (fungal) in aqueous solutions with different pH.

Changes in the optical properties of aqueous solutions of melanin were monitored over a pH range from 1 to 12. It was revealed that the solubility of melanin strongly depends on the pH. At pH = 1 melanin is practically insoluble in water while rising of pH the solubility of melanin increases.

Melanin has black color and in absorption spectra broad structureless band in the range of 200-900 nm is observed. At pH = 1 in the absorption spectra of melanin in the range of 200-300 nm appears structure - bands with maxima at 230 nm and 270 nm. At neutral and high pH absorption spectra remains structureless. In the luminescence spectra of neutral solutions band near 500 nm is observed. Increasing of pH to 12 does not affect the position of band or the intensity of luminescence. By reducing of the pH to 1 luminescence spectra changes fundamentally: drastic increase of the intensity of luminescence, while maximum of band shifts to the short-wave area - up to 460 nm. The nature of the investigated phenomena is discussed.

OPTICAL STUDIES OF FLAVIN-DEPENDENT ENZYME

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All cellular organisms need thymidylate (dTMP) for the replication of their chromosomes, as dTMP is required for the biosynthesis of dTTP, a building block of DNA. Cells can produce thymidylate either *de novo* from dUMP(2'-deoxyuridine 5'-monophosphate) or incorporate thymidine using thymidine kinase. The *de novo* pathway of dTMP synthesis requires a specific enzyme, thymidylate synthase, which methylates dUMP at position 5 of the pyrimidine ring. There are two pathways for thymidylate synthesis, each utilising a different thymidylate synthase enzyme: ThyA (EC:2.1.1.45) and ThyX (EC:2.1.1.148). Both enzymes convert dUMP to dTMP, but there is no sequence identity between the two enzymes, and their mechanisms of action differ. Only ThyX uses FAD (flavin-adenine dinucleotide) as cofactor. Because ThyX proteins were found in many pathogenic bacteria and not in mammals, they can be promising antimicrobial target.

The aim of the work was to study dUMP binding affinity by ThyX protein from the hyperthermophilic bacterium *Thermotoga maritime*. This protein is very stable at high temperatures which allows studying it in a wide range of temperature.

We used absorbance, steady state and time resolved fluorescence spectroscopy. Spectra were registered for samples in 50mM Hepes buffers with different salt concentration (0.05 - 500 mM NaCl) and in range of temperature from 293 K to 343 K.

ON THE EFFECTS OF GAMMA IRRADIATION ON THE INDUCED BIREFRINGENCE OF STRETCHED POLYMER FOILS

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The aim of our paper is to evidence the influence of gamma radiation on the induced birefringence of Poly (vinyl alcohol) stretched foils with different thickness. Thin foils of PVA with different thickness were prepared and dried without modifying their separation surfaces. The polymeric foils were irradiated from 15 minutes to 4 hours using a 60 CO source for Gamma radiation. The induced by stretching under heating birefringence of PVA films was measured with a Babinet Compensator. Physico-chemical processes (photo stabilization, photo degradation, oxidation) induced by irradiation of polymer matrix influence both the stretching degree and the anisotropy of etired foils. An increase of birefringence versus the stretching degree of the PVA foils was evidenced for all studied samples. The dependence of the birefringence on the films thickness was also confirmed. The induced birefringence of studied polymer foils was influenced by: stretching degree foils thickness and exposure time.

INFLUENCE OF UV RADIATION ON THE KINETICS OF GLUCOSE RELEASE FROM POLYMER FOILS

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The need of polymeric carriers permitting controlled release of a desired drug following oral administration has led to the screening of a large variety of synthetic and natural polymers. This paper reports the effects of UV radiation on *in vitro* evaluation of glucose release from the polyvinyl alcohol foils. The dependence of the glucose release profile from PVA is made for different exposure time (15 minutes to 6 hours) and for different drug content from the polymer matrix. The mechanism involved in drug release process is evaluated using Korsmeyer–Peppas empirical equation. The surface tension is determined by contact angle measurements using the sessile drop technique with four liquids and the changes induced by the glucose on the surface polarity are evaluated.

SPECTRAL PROPERTIES OF CHEMICALLY MODIFIED FORMS OF THIOFLAVIN T

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Thioflavin T (ThT) is widely used for the detection and study of the amyloid fibrils structure. The dye has low fluorescence quantum yield in aqueous solution, which increases by thousands of times when the dye is incorporates into amyloid fibrils. According to our data the main reason of this phenomenon is the rotational motion of benzothiazole and aminobenzoyl rings relative to each other in solution of low viscosity and restriction of this motion on ThT incorporation in amyloid fibrils. Photophysical properties of ThT are substantially determined by the methyl group at N5 atom of benzothiazole ring. The presence of this group not only prevents a planar configuration of the ThT molecule but also diminishes the energy barrier of internal rotation.

In this work two different analogues of the ThT, which differ from ThT by the lack of a methyl group at the nitrogen atom of benzothiazole ring were studied. It is shown that these analogues of the ThT, in contrast to the ThT, have significantly different pKa values characterizing protonation of the nitrogen atom of benzothiazole of the ring. In ThT pKa of this group lies in the alkaline pH range while the pKa of the ThT analogues is in acidic pH. In solutions with pH 2.0, which were used in our studies, there is probably a mixture of neutral and charged forms. The properties of cationic form are similar to those of ThT. It is shown that the absorption spectrums of the ThT analogues are significantly changed when they are bound to amyloids.

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SELF-ASSEMBLY OF TRICATIONIC MESOPORPHYRIN ON INORGANIC POLYPHOSPHATE SCAFFOLD

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Self-assembly of mesoporphyrins on different polymer matrices attracts essential attention of scientists due to their potential applications in nanomedicine and nanotechnology including design of nanodevices, fabrication of light-harvesting systems etc. *Meso*-substituted tris(*N*-methylpyridinium) porphyrin ($TMPyP^{3+}$) is a tricationic analog of tetracationic porphyrin TMPyP4, which can be easily functionalized, e.g. with a carboxyalkyl group, to allow the covalent attachment of other molecules. In recent years a conjugation of $TMPyP^{3+}$ with various ligands was used to achieve the selective stabilization of G-quadruplex structure of telomeric DNA [1], as well as for the development of efficient chemical nucleases and photocleavage agents of DNA. In the present work the self-assemblies $TMPyP^{3+}$ on the polyanionic inorganic polyphosphate (PPS) in aqueous solution were studied employing different spectroscopic techniques and DFT calculation method.

From the fluorescence quenching of the bound $TMPyP^{3+}$ molecules and their Raman spectra we conclude that porphyrin chromophores form the stable π-π stacking-assemblies onto PPS polyanions. The transformation of the Soret band in absorption spectra at different $TMPyP^{3+}$/PPS concentration ratios evidences that these assemblies are mixtures of *J*- and *H*-aggregates. Molecular modeling performed shows that the flexibility of PPS strand allows a realization of spiral or “face-to-face” one-dimensional structures formed by porphyrin molecules arranged in parallel and antiparallel mode. The peculiarity of PPS structure allows a formation of two porphyrin stacks on opposite sides of polymer strands that result in appearance of higher-order aggregates. The size of these aggregates was estimated from the light scattering data.

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SPECTROSCOPIC STUDY OF POLYMER METAL COMPLEXES BASED β-DIKETONES AND LANTHANIDES

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There has been a large research activity on coordination compounds of the lanthanide ions with organic ligands including *β*-diketones, which can act as excellent light conversion molecular device, light-emitting diodes, polymer sol–gel derived glasses, electroluminescent devices [1-3]. On the basis of the unique photophysical properties of lanthanide cations (long luminescence lifetime and very sharp emission band), rare earth metal complexes as luminescent materials have received increasing attention for application such as analytical sensors, imaging techniques, displays and organic light-emitting diodes [4,5].

We synthesised monomer – 2 methyl-5-phenylpentene-1-dione-3,5, their complexes with Sm(III), Lu(III), Tb(III) and phenanthroline, metallopolymers based of them. The synthesized compounds have been studied by NMR, IR-, electronic absorption and diffuse reflectance spectroscopy also thermal analysis as well as dynamic light scattering method and electron microscopy.

All compounds were studied by dynamic light scattering in order to determine particle size, as well as for solvent selection for the homogeneous thin films modeling. The size of monomer and polymer particles is virtually identical that is based on particle size distribution diagram.

The system is homogeneous in terms of uniform distribution of metal throughout the polymer matrix as seen from the micrographs of powdered samples and films.

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ELECTRON IMPACT EXCITATION AND IONIZATION OF NUCLEIC ACID BASE MOLECULES

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The main part of destructive changes at the molecular level of biostructures is connected just with slow electrons. In this case, the genetic macromolecules of DNA and RNA become the main target. Information about physical structure of molecules is necessary for understanding the roles of primary physical processes for functioning the biosystems and the influence of different environmental factors upon them.

The experiment is based on the method of crossed molecular and electron beams, which we have successfully applied earlier [1]. The electron beam was formed by the five-electrode gun with a tungsten cathode. The experiments were performed under the following conditions: the electron beam current was within (3-4)10^{-5}A and the electron energy spread (FWHM) being $\Delta E_{1/2} \sim 0.5$ eV, the vacuum degree in the chamber, where the cell with molecules steam was located, was ~1$10^{-5}$ Pa. Nucleic acid base molecules: uracil, thymine, adenine, cytosine and guanine are investigated. The experimental investigations of excitation and ionization of nucleic acid base molecules in gas phase by slow electrons are made. The emission and mass - spectra of molecules and their excitation and ionization functions are obtained.

As a result of our studies absolute values of the positive molecules ion production cross sections as well as their energy dependences were determined. The ions of the molecular fragments (dissociative ionization) are characterized by much smaller ionization cross sections, $\sim 10^{-17}$–10^{-18} cm^2. Among the fragments, relatively large ionization cross sections are typical of groups CNO, CH_2H_2, C_3H_3, C_2NH, and $C_2H_3N_2$, C_3H_3O, C_3H_5N, and C_3HNO. Ions of the fragments of a molecule without a side group $–CH_3$, as well as ions of a pyrimidine ring, are also observed. The photoemission (luminescence) spectra of molecules under the influence of electron impact in the wavelength range of 200–500 nm for different energies of electrons were experimentally obtained. almost all bands have complicated character, and it testifies to their superposition nature.

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ANTISYMMETRIC-ASYMMETRICAL EXCITATIONS IN *α*-SPIRAL REGIONS OF THE PROTEIN MOLECULE

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The proteins are the basic functional component of an organism. Structural changes in proteins - is the basis of changes in their functional properties, which are most often manifested in the form of diseases. Therefore, analysis of influence of structural characteristics of proteins on their conformation functioning, studying of their spatial organization, mechanisms of formation and activity of supramolecular complexes for medicine and biotechnology are remains actual.

In this paper we consider the classical model of *α*-helix as a one-dimensional molecular crystal with three molecules in the unit cell. Different types of conformation responses α-spiral region of a protein molecule on excitations are analyzed. In the hydrolysis of ATP occurs intramolecular quantum excitation. The nonlinear response of an α-spiral region of a molecule to this excitation was considered. It was found that in the simplest case, three types of excitations are realized: symmetrical, antisymmetric and asymmetrical.

Here we focused on the latter two types of excitations.

Antisymmetric exaltations, most likely, are realized in membranous and nucleic proteins. At such excitation one of peptide chains does not change, while the other two are shorten. This asymmetry leads to that the *α*-spiral region takes the form of a curved segment of a torus instead of the cylinder. It is shown, that in many membranous and nucleic squirrels the conformation response of *α*-spiral region of the protein compounds quantity of order $N_c/5$ (in angstroms), where N_c is number of spiral turns. For number of turns typical in this case: $N_c \sim 10 \div 15$, the displacement, it seems, is of the order of $2 \div 3$ angstroms. It qualitatively corresponds to observable values.

Asymmetric excitations, most likely, are realized in enzymatic proteins. The energy of the asymmetric excitation is less, than antisymmetric. At such excitations one of three peptide chains of α-spiral is shortens more than the other two. It is shown that in this type of excitation the bending of the α-spiral formally directed in opposite side with respect to antisymmetric excitations. Also it has a greater value than in the antisymmetric case if $N_c \leq 14$ and smaller if $N_c > 14$. All of this allows us to consider the combined antisymmetric-asymmetrical excitations for the interpretation of complex movements of α-spiral regions of the protein.

SYNTHESIS OF BENZYLIDENE AND AZO CONTAINING POLYMERS FOR PHOTOPHYSICAL APPLICATION

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The development of modern technologies enables us to create polymer materials with a number of properties, which would be impossible to realize in a single polymer. Also it should be noted, that in the last few years there has been a growing research interest in developing materials which exhibit nonlinear optical (NLO) properties for applications such as optical signal processing and information storage [1,2]. In this work, our investigation concentrates on synthesis of new oxazolone, thiazolidenone, thiohydantoin, hydantoine and azo- derivatives radical thermoinitiated copolymerization of new methacrylic monomers with methylmetacrylate. The aims of our work were synthesized polymers with photochemical properties typical for single molecules. Polar substituents in azobenzene compounds and nature of heterocyclic fragments in benzyliden containing derivatives lead to the change of electronic density during the photoisomerisation. This fact opens the possibility of creation polymer materials with predicted properties.

During the work new objects for NLO investigation were synthesized. The polymers with MMA with benzylidene and azo fragments were obtained. The polymerization ability of the new monomers was investigated kinetically for radical copolymerization using the dilatometric method. The azo polymers have been characterized as compound with repeatable *trans-cis-trans* isomerisation process, for the benzylidene containing polymers we can observe *cis–trans–cis* isomerization cycle. These polymers can prove to be important candidate for optical signal processing and information storage.

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THE UNFOLDING-REFOLDING OF iRFP DERIVED FROM BACTERIAL PHYTOCHROME

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Bacterial phytochromes (BphPs) have attracted attention recently as they can be used to construct novel fluorescent probes for bioimaging of living cells and tissues for highly versatile biological applications and medical diagnostics. An optimal fluorescent probe for imaging in tissue should have both excitation and emission spectra in a near-infrared “optical window” (NIRW: ~650-900 nm) where mammalian tissues are the most transparent to light. Recently such fluorescent probes have been developed on the basis of BphPs, including iRFP, IFP1.4. In these probes biliverdin IXα (BV), which is a natural ligand of BphPs, is used as a chromophore. As BV is a component of endogenous mammalian heme metabolism, no exogenous cofactor is needed. Despite the importance of BphPs, little is known on photochemical processes underlying their near-infrared fluorescence and the amino acids stabilizing different chromophore states. The folding of BphPs containing the rare knot structure between domains involved in chromophore binding has not been investigated also.

In this work we studied the guanidine hydrochloride induced denaturation-renaturation of iRFP in apo and holo-form using spectroscopic techniques (absorbance, fluorescence, circular dichroism). It was shown that the denaturation of iRFP in apo-form (without BV) is fully reversible as indicated by the recovery of all recorded parameters. The chromophore binding increases the protein stability and denaturation cooperativity but makes the denaturation of iRFP in holo-form irreversible as its renaturation is complicated by aggregation of partially folded protein molecules.

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COMPLEX ENERGY LANDSCAPE OF DIMERIC BOVINE ODORANT-BINDING PROTEIN

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Despite an increasing number of studies on the stability and unfolding processes of proteins with β-barrel topology, these processes have been understood to a much lesser extent than for α- and α/β-proteins. A large group of odorant-binding proteins (OBPs) share a common nine-stranded β-barrel structure which encloses a ligand binding site composed of an internal cavity and an external loop scaffold. Investigation of OBPs is also important due to their possible use as sensitive elements of optical biosensors for dangerous substances such as toxic, explosive and so on. Exposure resistance must be an important characteristic of any proteins which can be regarded as a potential sensitive element of any biosensor system.

This work is focused on the study of dimeric bovine OBP (bOBP) which in contrast to classical OBPs is characterized by a unique folding pattern that involves the crossing of the α-helical domain of each monomer over the β-barrel of the other.

In this work we studied the guanidine hydrochloride (GdnHCl) induced denaturation-renaturation of recombinant bOBP using spectroscopic methods and size-exclusion chromatography. It was shown that the recombinant bOBP possesses high resistance to denaturing action of GdnHCl. We revealed that formation of two native-like states of bOBP precedes the complete unfolding of the protein globule. These local changes of bOBP in the region of pre-denaturing GdnHCl concentrations did not result in alteration of the protein capability to bind ligand.

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THIOFLAVIN T INTERACTION WITH ALPHA-SYNUCLEIN AMYLOID FIBRILS

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Formation of ordered aggregates - amyloid fibrils - is associated with the occurrence of many serious diseases such as Alzheimer's, Parkinson's, prion disease, type II diabetes, etc. Despite the great interest in this issue, the processes underlying the abnormal protein aggregation and its pathological manifestations in the disease are poorly understood. The successful solution of these problems depends on the fundamental knowledge of the structure and properties of amyloid fibrils.

The aim of this work is the investigation of alpha-synuclein amyloid fibrils depositions of which accompanies Parkinson's disease. The main tool for the comparative study of the structure of amyloid fibrils used in our work is the fluorescent dye thioflavin T (ThT). To study the interaction of this dye with amyloid fibrils, we developed a special approach based on the absorption and fluorescence spectroscopy of solutions obtained by equilibrium microdialysis [1,2]. With the use of this approach it was defined ThT-amyloid fibrils binding parameters and the characteristics of the bound dye. The estimated parameters were analyzed in comparison with the existing information about ThT binding to insulin, lysozyme, Abeta-petptid, and beta-microglobulin amyloid fibrils [3]. Obtained results confirm the notion that the fibrils on the basis of different proteins are distinct and that proposed approach can be used to compare and study of their structure.

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THERMODYNAMIC PARAMETERS Zn^{2+}, Ni^{2+} AND Co^{2+} ION BINDING WITH DNA BEING IN METALLIZED FORM

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Studies carried out in the last years revealed that in alkaline solutions (pH 8-9) ions of transition metals induce B-DNA transition into a new double-helical conformation (m-form) being of metallic conductor properties. Together with technological tasks of the polynucleotide m-forms application as nanoelectronics elements, their peculiar properties are of interest for biophysics too.

Methods of visible and differential UV-spectroscopies and thermal denaturation were used to determine Zn^{2+}, Co^{2+} and Ni^{2+} ion binding constants to bases of metallized DNA in alkaline solutions of different contents and enthalpy of the B→m transition.

The most efficiency of DNA metallization with Zn^{2+} ions is caused by the fact that the constant of m-form creation with these ions is by (2-3) times higher than that for Co^{2+} and Ni^{2+} ones. It is shown that corresponding to the formation of interstrand metallic bridges in complementary DNA pairs, the constant of Zn^{2+} ion binding is higher than that characterizing the formation of coordination bonds with heteroatoms of nitrogen bases of single-stranded DNA. This is just condition that ensures an additional increase in the thermal stability of the double-stranded DNA upon its transition from B-form to m-one. Induced with Zn^{2+} ions, a larger (by module) change in the temperature of the cooperative B→m transition (- 28 °C) (in comparison with the temperature change of m→coil transition (+ 10 °C)) is conditioned not only with differences in binding constants of Zn^{2+} ions to bases of B- and the single-stranded DNA forms but with differences in enthalpies of these transitions.

SPECTROSCOPIC STUDIES ON COMPETITION BETWEEN TWO DNA-QUINACRINE BINDING MODES

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Binding of acridine derivative quinacrine (QA) to chicken erythrocyte DNA was studied by methods of absorption and polarized fluorescent spectroscopy. Measurements were carried out in aqueous buffered solutions (pH 6.9) of different dye concentrations ($[QA] = 10^{-6} \div 10^{-4}$ M) and ionic strengths ($[Na^+] = 10^{-3} \div 0.15$ M) in a wide range of phosphate-to-dye molar ratios (P/D). It is established that the minimum of fluorescent titration curve plotted as relative fluorescence intensity vs P/D is conditioned by the competition between the two types of QA binding to DNA which posses by different emission parameters: (i) intercalative one dominating under high P/D values, and (ii) outside electrostatic binding dominating under low P/D values, which is accompanied by the formation of non-fluorescent dye associates on the DNA backbone. Absorption and fluorescent characteristics of complexes formed were determined. The method of calculation of different binding modes contribution to the complex formation depending on P/D value is presented. It was shown that the size of binding site measured as the number of DNA base pairs per one QA molecule bound in the case of the electrostatic interaction is 8 times less than that for the intercalative one that determines the competitive ability of the outside binding against the stronger intercalative binding mode.

9

METHODS AND APPLICATIONS

NEW METHOD FOR DETERMINING THE DISPERSION OF A POLYMER SOLUTION OPTICAL ACTIVITY

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The proposed method is based on the channeled spectra recorded for an anisotropic polymer solution placed between two crossed polarizers. The collimated light beam is linearly polarized when it passes through the polarizer and suffers dispersive rotation of the polarization plane. The emergent beam from the analyzer is recorded with a spectrophotometer. A channeled spectrum, whose structure depends on the specific rotation, its dispersive properties and also on the thickness of the solution layer, allows to determine the specific rotation, the dispersive parameter and the channels orders only by solving an equation system in which the conditions for two consecutive channels and the maximum between them are written. Finally, the parameters of the interest are written as functions on the wavelengths in the consecutive minima and maxima of the channeled spectrum, on the thickness of the solution layer and also on the solution concentrations.

The results were obtained for propyl-cellulose solved in methanol.

UPGRADING THE SPECTRAL COMPUTING UNIVERSAL COMPLEX

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The facility called KSVU-12 (spectral computing universal complex) can be used for investigation of LEDs [1] or crystals. For example, the «green» GaP LEDs were studied with it. The investigation of nitrogen alloyed GaP-LEDs was performed at «liquid nitrogen» and «ambient» temperatures [2]. The apparatus comprises diffraction grating with 1200 lines per mm, photomultiplier PMT-100 at voltage U = 1.2kV, thus features scan speed 100 nm/min with step of 0.1 nm.

Optical scheme of this complex is very reliable and enduring, and it was used for spectroscopic measurements and education at the Department of Experimental Physics (Faculty of Physics) for over two decades (the production is dated back as 1988). The performance optical part of the instrument is rather satisfactory, while the receiving channel and the data acquisition and processing subsystem is obviously outdated. The complex is managed via micro-computer «Electronika MS-1201,» at performance of (400 ± 100) instructions per second, with loading OS RAFOS out of floppy disks. Recently, frequent failures occur, sometimes the system does not even boot. Data acquisition channel is implemented on the basis of photo-electronic multiplier, that results in additional difficulties of digitization and processing.

Due to the drop in prices for computer and electronic components, and emergence of open hardware (eg, Rasberry Pi [3]), the perspective of the revival of the instrument looks very promising. Also, the full automation based on GNU/Linux, with subsequent data visualization is to be implemented.

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COMPACT-SIZED BATTERY POWERED EXCIMER LASER FOR SPECTROSCOPIC INVESTIGATION IN FIELD CONDITIONS

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Compact sized excimer laser with dimensions 300x230x100 mm3, low weight 8-10 kg and battery powering is designed. Laser generates at typical excimer gas mixtures. Output energy when generating at 308 nm is 5 mj, repetition rate is a few pulses per second. Above advantageous in combination with compact spectrometers allow one to conduct optical and spectroscopic investigation in really field conditions.

The possibility of spectral - for example Raman - experimental measurements practically in any field conditions opens up tremendous opportunities for quick, prompt research environment: water, vegetation, atmospheric objects. That in turn will not only deepen the knowledge about the environment and the processes in it, but also will allow us to track the impact of human activities on the environment.

CONTROL OF THE FUNCTIONAL STATE OF ONE-CELLED ALGAE IN SUSPENSIONS BY LUMINESCENT METHODS

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Possibility of using the luminescence methods for the state diagnostics of one-celled algae in liquid medium is analyzed. Application of conventional method of fluorescence induction is shown to be difficult due to possible mixing the liquid in the measurements. However, the diagnostics can be made by measuring the static intensity and luminescence spectra of chlorophyll *a*.

The functional state control can be realized by such luminescent parameters as the efficiency of chlorophyll photoluminescence or the ratio of the intensities in the characteristic emission peaks of this pigment. It is concluded that the total photoluminescence intensity of chlorophyll divided by the concentration of individuals in the suspension can be used as the relative efficiency of luminescence when the cell number in the culture is small and the absorption of excitation light is insignificant. When the absorption and scattering are considerable, calculation of the mentioned efficiency becomes more complicated.

It is shown that the results of measurements can be greatly distorted by the fluorescence induction effect. To minimize this effect, the regular interchange of the cells under excitation beam is proposed, which allows each of them obtain a relatively small exposure dose.

Advantages of low-temperature measurements are discussed. It is stressed, herewith, that the excitation wavelength should be surely taken into account because the control luminescent parameters can behave differently depending on whether the excitation of the chlorophyll *a* luminescence is direct or it is sensitized.

Taking into account a strong dependence of the luminescent parameters of the plants on external conditions, the diagnostics of the functional state of the object should be performed in comparison with the reference sample.

SUB-DOPPLER FREQUENCY-MODULATION LASER SPECTROSCOPY OF MOLECULAR IODINE IN EXPANDED SPECTRAL REGION NEAR 640 NM

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The precise frequency locking of laser onto the iodine hyperfine transitions is widely used in laser metrology and laser spectroscopy (for example, it one can use for the determination of the nuclear electric quadrupole interaction and the nuclear spin rotation interaction parameters of iodine molecule). The very promising set of iodine $^{127}I_2$ transitions for laser frequency stabilization includes the wavelengths 515 nm (a_3 component P913)43-0), 532 nm (a_{10} component R(56) 32-0), 576 nm (a_1 component P(62) 17-1), 611 nm (a_7 component R(47) 9-2), 633 nm (a_{16} component R(127) 11-5), 640 nm (a_9 component P(10) 8-5). Here we introduce the frequency-modulation saturated absorption spectroscopy for study of hyperfine structure of iodine $^{127}I_2$ absorption lines R(25) 8-5 and P(19)8-5. The important feature which we use in our approach is that the FM-resonances are a sum of individual resonances shifted on half of the modulation frequency what gives the frequency reference. The frequency reference given by the value of the modulation frequency as frequency marker allows the determination of the frequency difference between hyperfine components.

The external cavity diode laser has been used for realization of experiments on frequency-modulation saturated absorption spectroscopy of molecular iodine. Spectral range of laser generation is 638 – 642 nm, output power – 40 mW. Within the tuning range of the laser more than 1000 strong rovibronic lines of the $^{127}I_2$ molecules can be observed. Frequency modulation of the laser output radiation is produced by modulation of the laser diode injection current with frequency 12.5 MHz. The signal from the photodiode is operated on the digital lock-in amplifier.

The hyperfine structure of iodine absorption lines R(25) 8-5 and P(19)8-5 was recorded. The frequency reference given by the value of the modulation frequency (12.5 MHz in given experiment) allows determination of the frequency differences between hyperfine components with accuracy better than 0.1 MHz using the fitting procedure in experiment with only one laser.

Due to the external cavity diode laser ability to tune of single-frequency output into wide spectral region, the high-resolution iodine spectra was recorded in the frequency region more than 20 GHz.

THE POSSIBILITIES OF THE COLORIMETRIC METHOD FOR MEASURING OF WAVELENGTH'S DISTRIBUTION OF LIGHT RADIATION IN USUAL AND THE RAW FORMATS

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The possibilities of colorimetric measurements of the wavelength's distribution of light emission for usual [1] and RAW formats [2] are compared in this work. The need in such measurements appears when using holographic sensors. The wavelength of radiation, registered at this point, can be uniquely defined for the narrow-band radiation on the interval of the monotone dependences of color hue on the wavelength at any point of digital image.

For working of the method it is necessary to calibrate the camera. It was found that in usual formats the color hue depends not only on the wavelength but also on the intensity. In RAW-format this dependence is practically absent. The spectral response of the camera was studied and calibrated by incandescent lamp's spectrum. The obtained characteristics allow us to define the wavelength of the radiation acting on this pixel through the color hue of a pixel and its brightness.

Camera Sony F717 was used while working in the usual format, camera Canon EOS 10D was used in RAW-format. In a usual format their characteristics were qualitatively similar, only the values of operating limits were different. There are two operating ranges in a usual format for the working camera: 570-605 nm and 450 - 535 nm. In RAW-format the working range is expanded to the range of 455 - 625 nm. In the spectrum of the incandescent lamp the standard deviation is mainly 0.3-2.0 nm, depending on the wavelength. The method was used to analyze the various components at different points in space and in various states of holographic sensors at different points, including the measurement of glucose in serum.

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STATIC AND DYNAMIC EFFECTS IN BINARY CHIRAL SYSTEMS

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An interest in studying the properties of optically active substances and their mixtures increases every year. In particular, the needs of medicine and pharmacology are in synthesizing new substances which in most cases are optically active. On the other hand a quality control of natural origin also requires determining the relative content of chiral compounds.

To determine the relative content of OA substances in a binary system we have chosen the method of determining the optical activity of the three known wavelengths. We have implemented the method of computer modeling for determining the relative content of glucose and fructose in their binary chiral system. So we have solved the inverse static (in time) problem of polarimetric binary systems.

Considering the effects of mutarotation processes binary chiral systems (under certain conditions) may have fluctuating nature, i.e. time depending nature of polarization's plane azimuth of the output binary system which are fluctuating in the nature (a phenomenon similar to the known reaction of Belousov - Zhabotinsky). Computer simulation results have confirmed our hypothesis. [1]

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SYNTHESIS OF GRAPHENE BY MAGNETRON SPUTTERING USING HYDROGEN AS PLASMA-FORMING GAS

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Synthesized single and multilayer graphene films by magnetron sputtering using a graphite target and hydrogen as plasma-forming gas. For the substrate used Ni-Fe foil, which was heated by passing an electric current. Using Raman scattering method, found the conditions formation of monocrystalline graphite layer, single-and multi-layer graphene. From the data of micro Raman scattering it follows that synthesized uniform graphene films (up 180mkm) have high quality - practical absence of D band (~1350 cm^{-1}) and the ratio of band intensities 2D (~2705 cm^{-1}) to G (~1580 cm^{-1}) reaches 7.4.

BEER LAMBER LAW IN PHOTONIC CRYSTAL SPECTROSCOPIC STUDY

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Photonic crystals with defect of periodical structure can be used as optical filter for NDIR-spectroscopy. Due to the long effective length of the radiation propagation in photonic crystal fiber (PCF) sensor sensitivity can be improved [1]. For guided modes of the PCF effective propagation length can exceed fiber length. Attenuation of guided modes is not the same as power absorption in host glass.

In our work PCF transmission was calculated by using biortiogonal mode field decomposition. PCF modes are obtained from vectorial Helmholtz equations for transverse component of magnetic fields vector. [2] Plane wave expansion method was used. We introduced right and left eigenvectors

$$\begin{aligned} \mathbf{M}\cdot\mathbf{r}_i &= \beta^2\mathbf{r}_\mathbf{i} \\ \mathbf{v}_\mathbf{j}\cdot\mathbf{M} &= \beta^2\mathbf{v}_\mathbf{j} \end{aligned} \qquad (1)$$

where $\mathbf{r}_\mathbf{i}$,$\mathbf{v}_\mathbf{j}$ - right and left vectors, containing Fourier components of H_x, H_y fields. **V** and **r** vectors are biortogonal, which allows us to expand inner field of the PCF using biortogonal conditions, □ – mode propagation constant (tangential component of the wave vector).

The used method can be applied for the calculation of fiber transmission in photonic crystal bandgap. The proposed method calculates the transmission of a single-mode and multimode PCF with the vector nature of the guided modes field consideration. In practical application, this method of calculating PCF modes and light propagation can be used in spectroscopic applications and gas or liquid media sensors development.

Results, obtained by the method are:

1. Power absorption coefficient is variable within the bandgap of PCF
2. The concentration of the media studied by PCF NDIR spectriscopy via Beer-Lamber Law was evaluated.

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HOLOGRAPHIC GLUCOSE SENSORS – KINETICS OF THE RESPONSE

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Hydrogel holographic sensors are a new kind of optical sensors, potentially suitable for the analysis of aqueous solutions and components of gas mixtures.[1,2] The principle of operation of such sensors is based on the change in the period of the holographic grating recorded in the hydrogel matrix that swells or shrinks in the presence of the analyte mixture. These changes are accompanied by corres-ponding changes in the wavelength of the reflected light, which is easily detected using a fiber spectrograph.

Holographic glucose sensors were synthesized in the hydrogel matrix consisted of three-dimensional polymer net of acrylamide (AA), N-acryloyl-3-aminophenylboronic acid (AMPh), (6 mol.%), N-acryloyl-D-2-glucosamine (NGA), (6 mol.%) and N,N'-methylene-bis-acrylamide (bis), (0,5 mol.%) grafted on glass plate. Holographic gratings was formed in hydrogels as a result of the interference between the incident and the reflected beam (from a mirror placed behind the hydrogel) when irradiated by the red He-Ne laser (632,8 nm, power - 15 mW)[3] or green laser pointer (532 nm, 1,5 W).

The rate of optical response exhibited by a holographic sensor to the changing concentration of analyte is important characteristic determined by the rate of sugar diffusion into the gel as well as by the rate of affinity complex formation and structural rearrangements of the gel due to the increasing concentration of negative charges resulting in gel hydration and swelling. Affinity complex formation between the sugar and PBA groups, or structural rearrangements of the gel due to its enhanced hydration in the presence of binding sugar seemed to input the rate of optical response

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STRONTIUM AND CALCIUM RELATIONS IN PLANT AND SOIL SOLUTION ON CHORNOBYL AFFECTED AREAS

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Ratios Sr/Ca for natural total strontium and ^{90}Sr/Ca in plants and in the corresponding soil solutions for three experimental lands with “fuel” type of pollution for several plants at natural conditions are determined. Content of Sr and Ca at the samples were determined with optical ICP spectrometer. Content of ^{90}Sr at the samples were determined with radiochemistry. These lands with three different types of soil are at the Exclusion Zone of the Chornobyl Power Station. The obtained experimental results show that ratio Sr/Ca in plant is equal to this ratio in the corresponding soil solution for all investigated lands and plants. Ratio ^{90}Sr/Ca in plant exceeds this ratio in the corresponding soil solution. The ratio in the plant has positive correlation with the soil humidity for every experimental land.

DESIGN OF DYE-SENSITIZED SOLAR CELLS WITH VARIOUS METHODS OF FORMING LAYERS ZnO

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One of the most promising ways to increase the efficiency of dye-sensitized solar cells with various methods of forming layers of ZnO is a purposeful method of forming a semiconductor layer topology, which provides increased trajectory of scattered photons in this layer.

Due to the so-called ‘Pop-Corn Ball Effect’ experimentally registered a double increase efficiency. This was achieved by forming layers with a diameter of 300 microns (on which scattering happens). They consist of smaller - diameter of 20 nm.

Promising method of forming the desired topology layer of ZnO is proposed [1] required (hierarchical) structure. In our work we have a large number of samples to compare the effectiveness of different methods of cell manufacturing semiconductor layers.

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LASER-INDUCED INCANDESCENCE OF CARBON SURFACE

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Irradiation of light-absorbing objects by powerful pulsed lasers can produce thermal emission in the visible spectral range. This emission is called LII (laser-induced incandescence). LII is usually observed with black microparticles or surfaces under irradiation by a nanosecond-timescale laser radiation of moderate power density. Properties of LII of surface layers are of interest for possible applications as a factor of monitoring of temperature in pulsed-laser processing of surfaces.

In this work, (LII) of carbon surface is investigated under 1.06 μm YAG:Nd^{3+} pulsed laser excitation. The experiments show that the intensity of LII of carbon surface depends on the initial (before the laser irradiation pulse) temperature T_a of the investigated sample. With the increase of T_a the intensity of LII I_{LII} increases significantly. For example, the increase of T_a from 300 K to 350 K leads to the increase of LII signal by approximately 25%. With taking into account this property of LII, a new method is proposed for estimation of temperature of laser-heated surfaces.

The method requires measurement of LII at a fixed wavelength λ with application of a moderate variation of initial sample temperature ΔT_a. Maximal value of laser-induced transient of surface temperature can be estimated with the use of the following expression

$$T_m = \sqrt{\frac{hc}{\lambda k_B} \cdot \frac{I_{LII}}{\Delta I_{LII}} \Delta T_a}$$

It should be mentioned that the proposed method of surface temperature estimation is based on the supposition that the maximal surface temperature linearly increases with the laser power. The validity of this supposition is substantiated by the appropriate computer simulations. These simulations are based on the model which assumes that the laser-heated surface layer losses its internal energy through thermal conduction into the bulk sample.

COHERENT PROPERTIES OF FEMTOSECOND SUPERCONTINUUM FOR SPERCTROSCOPY PURPOSES

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Usage of femtosecond supercontinuum (SC) in spectroscopy systems was studied actively since beginning of XXI century. But this application needs some very specific parameters of output signal, such as high degree of coherence. Hence investigation of SC coherence properties and possibilities of its improvement is very actual.

Aim of this work is analysis of SC coherence generated by high intensity ultrashort pulses in microstuctured fibers. Spectrum of this SC type has self-shifted solitons (SSFS) in IR region which is the reason of SC coherence degradation.

For this purposes we calculate coherence degrees for experimental results and theoretically modeled results. Results show SC strong coherence degradation in blue and IR region caused by amplification of Raman gain. But visible range spectrum show satisfying results for spectroscopy goals. That correlates with previous investigation studies carried out by our group of researchers.

Also at summer school will be presented calculation of spatial and spectral coherence properties of femtosecond SC.

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COMPUTER SIMULATION

AB INITIO MODELING OF THE STRUCTURE AND ENERGETIC PARAMETERS IN CHAIN AND RING CLUSTERS OF ALCOHOLS

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Alcohols are specific kind of substances which molecules can combine into relatively stable cluster structures due to capability of forming hydrogen bonds. The size and shape of clusters and consequently the properties of alcohols connected with the strength of hydrogen bonding, which, in turn, dependent on the nature of alcohols i. e. the length and shape of the dispersive alkyl backbone.

The aim of the present research is to trace the dependence between the hydrogen bonds strength and the size of the alcohol molecule backbones in the different cluster structures. The stability of cluster structures was evaluated by the amount of total energy per molecule. In the case when room temperature (298 K) is considered the entropy affects were accounted and the enthalpy and free Gibbs energies of interaction were compared for different clusters.

As objects of investigation the methanol, ethanol, 1-propanol, 1-butanol, and 1-pentanol were chosen. The energies of different chain-like and ring clusters comprising from 2 to 6 molecules for each alcohol were calculated and the comparison with the experimentally registered spectra was made.

The calculated IR spectra of the most profitable structures were compared with the experimental ones registered at different temperatures.

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INTERPRETATION OF IR AND RAMAN SPECTRA OF 4,4'-CHLOROBENZOPHENONE BASED ON MOLECULAR MODELING BY METHOD OF DENSITY FUNCTIONAL THEORY

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Vibrational IR and Raman spectra of 4,4'-chlorobenzophenone (4,4'-ClBP) have been measured at room temperature. Modeling of the structure and vibrational spectra has been performed. Energy, structure, dipole moment, polarizability, force constants, frequencies of normal modes in harmonic approximation and their intensities in the IR and Raman spectra have been calculated. Modeling 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. Process of scaling has been used for decrease of the discrepancy between calculated frequencies in harmonic approximation and measured frequencies.

66 normal modes of molecule 4,4'-ClBP are divided into equal parts between two symmetry types C2 point group: a and b. In accordance with the symmetry selection rules normal vibrations both symmetry types are allowed in the vibrational IR and Raman spectra of the molecule. Given the assignment of frequencies of the normal vibrations and preliminary interpretation IR and Raman spectra of 4,4'-ClBP.

Based on simulation results, we can conclude the applicability of the DFT method, using functional B3LYP and Basis 6-31G(d) to calculation of the structure of 4,4'-ClBP molecule and vibrational spectrum in harmonic approximation.

EXHIBITION OF INTRA- AND INTERMOLECULAR INTERACTIONS AND CONFORMATIONAL MOBILITY AT IR SPECTRA OF SALOL

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The IR spectra of salol have been measured by wide range of temperatures. Measurements can be held at a glass state or at two possible crystal states. Spectra measured at temperatures from 10 to 310 K differ from each other. What is the reason of the difference? We suggest that the conformation of salol molecule can differ with the difference of the temperature and phase state.

Conformational mobility of the molecule and intra- and intermolecular interactions is the reason of the differences that can be seen at spectra. To check the suggesting we hold the modeling of the conformers and their H-complexes and calculate their vibrational spectra. Conformers we had modeled differ from each other by the angles of rotation across the single bond C_8-O_{10}. The calculations were held by program complex GAUSSIAN 03 using the DFT method B3LYP functional in basis 6-31G(d).

Energies, structures, mechanical and electrooptical parameters and vibrational spectra of the molecular systems have been calculated. Using the results of the calculations the vibrational spectra of salol at crystall state modifications and glass state measured at different temperatures were interpreted.

IR SPECTROSCOPY AND QUANTUM MECHANICAL METHODS FOR INVESTIGATION OF CONFORMATIONAL MOBILITY OF BEHENIC ACID MOLECULE

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IR–spectrum of behenic acid $CH_3(CH_2)_{20}COOH$ were measured in a wide temperature range (11-330K). At higher temperatures spectral changes were revealed (bands shift and emergence of new bands, transformation of their forms and redistribution of intensity). Changes can be explained by molecular structure change in polymorphic transformations.

To confirm the assumption about the conformational mobility of behenic acid the structure and spectra of different behenic acid dimers, formed by hydrogen bonds were simulated. Barrier to rotation around the nearest to the carboxyl group C-C bond is about half of the barrier to rotation around the other C-C bonds, so the deformation of the molecule is most likely near the dimer ring.

Selected for modeling dimers differ by alkyl radical (AP) orientation relatively the carboxyl group and by orientation of fragment containing carboxyl group and closest to it CH_2-group relative to the rest of AR. The angles of rotation relative to the closest to the carboxyl group carbon bonds were taken in the range of 3-10°.

Simulation is carried out by DFT method (B3LYP/6-31G(d)). Energy were minimized, structures, dipole moments, polarizability, the normal frequencies in the harmonic approximation and the distribution of intensity in the IR spectra were calculated. The interpretation of the IR spectra were given.

On the basis of the calculated and measured IR spectra we made the conclusion about the conformational mobility of the behenic acid molecules, vibrations that are most sensitive to rotation relative to the closest to the carboxyl group carbon bonds, were identified.

TDDFT CALCULATIONS OF ELECTRONIC SPECTRA OF BENZOXAZOLES UNDERGOING EXCITED STATE PROTON TRANSFER

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Excited state proton transfer (ESIPT) has been extensively studied both experimentally and theoretically regarding its importance as a photochemical reaction as well as relevance for various applications. 2-(2'-hydroxyphenyl) benzoxazole (HBO), 2,5-bis(2-benzoxazolyl)phenol (DBP) and 2,5-bis(2-benzoxazolyl)hydroquinone (BBHQ) are benzoxazole derivatives that exhibit ESIPT from the hydroxy group to nitrogen atom, the tautomers are enol and keto structures [1, 2].

Energies and oscillator strengths of vertical transitions for various rotameric and tautomeric species of HBO, DBP and BBHQ have been calculated in the ground and first excited states with the use of TDDFT methods. The TDDFT results demonstrate good correspondence to the frequencies of absorption and fluorescence bands of the benzoxazoles reported for measurements in supersonic jets and solution, but fail to predict relative energies of enol and keto tautomers of DBP and BBHQ in the excited state. Low intensity of the fluorescence bands attributed to the conformations of HBO and DBP that do not undergo excited state proton transfer is shown to be caused by low concentrations of the conformations in the ground state. The enol conformations with OH...O hydrogen bonds have been calculated to exhibit blue shift of the first absorption transitions in relation to those of the most stable OH...N enol structures. For the three substances large-amplitude twisting of the keto tautomers has been found to be one of radiationless processes resulting in decrease of the fluorescence with a large Stokes shift [3].

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AB INITIO STUDY OF THE 4 $^2\Gamma$ STATE OF TRIATOMIC RARE GAS HALIDES

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This contribution reports on *ab initio* study of Rg_2X molecules (Rg – rare gas atom, X – halogen atom) with an emphasis on the lowest bound $4^2\Gamma$ state which is the source of broad band emission of halogen doped Rg gases and cryogenic Rg solids. The equilibrium geometry of $Rg_2X(4^2\Gamma)$ is isosceles triangle. Along the RgX-Rg bond $Rg_2X(4^2\Gamma)$ correlates with the ion-pair $RgX(C\ ^2\Pi_{1/2})$ state and with the ground state of Rg_2^+ ion along the Rg_2-X bond. Calculations were performed using MOLCAS [1] on RASSCF/CASPT2 level with inclusion of the spin-orbit interaction. Similar calculations were also performed for Rg_2^+ and RgX molecules using the same method and basis sets as for Rg_2X to obtain reference results for comparison. Table 1 shows bond lengths and vibrational frequencies for $RgX(4^2\Gamma)$ and for the forementioned states of diatomic fragments. As is seen the equilibrium $R_{Rg\text{-}Rg}$ distance in $Rg_2X(4^2\Gamma)$ is the same as in Rg_2^+ (X) whereas the $R_{Rg\text{-}X}$ bond is ≈ 0.2 Å longer than in RgX(C). The Rg-X bond elongation is the same for all Rg_2X independently of the bond length, which varies from 2 Å for NeF and up to 3.6 Å for XeI. Another interesting result concerns with $Rg_2X(4^2\Gamma)$ vibrations. The bending mode frequency remain close to v_e of $Rg_2^+(X\ ^2\Sigma^+_u)$ (Table 1) implying weak coupling with the symmetric stretch mode. Very similar result was obtained for triatomic alkali halides [2]. Dissociation energy and dipole moment of transitions coupling $RgX(4^2\Gamma)$with lower lying valence states have also been calculated in the course of present study.

Table 1. Internuclear distance (Å) and vibrational frequency (cm^{-1}) in the ground electronic state of Rg_2^+, the ion-pair state $C\ ^2\Pi_{3/2}$ of RgX, and the $4^2\Gamma$ state of Rg_2X. RASSCF/CASPT2 calculations, ANO-RCC-VQZP atomic natural orbital type basis set.

	Rg_2^+ X $^2S^+_u$		**RgX C $^2P_{3/2}$**			**Rg_2X $4^2\Gamma$ ($^2B_2$)**					
	$R_{Rg\text{-}Rg}$	v_e		$R_{Rg\text{-}X}$	v_e		$R_{Rg\text{-}X}$	$R_{Rg\text{-}Rg}$	v_a	v_s	v_b
Ne_2^+	1.71	591	NeF	2.00	526	Ne_2F	2.18	1.71	254	384	606
Ar_2^+	2.38	311	ArF	2.25	401	Ar_2F	2.46	2.36	165	293	345
			ArCl	2.76	265	Ar_2Cl	2.97	2.37	109	202	322
Kr_2^+	2.68	191	KrF	2.35	355	Kr_2F	2.56	2.64	164	293	199
			KrCl	2.88	223	Kr_2Cl	3.08	2.65	105	177	206
			KrBr	3.04	161	Kr_2Br	3.24	2.65	75	125	201
Xe_2^+	3.05	132	XeF	2.44	345	Xe_2F	2.65	2.94	198	349	165
			XeCl	2.99	206	Xe_2Cl	3.2	3.00	94	179	143
			XeBr	3.16	143	Xe_2Br	3.36	3.00	71	115	148
			XeI	3.39	115	Xe_2I	3.62	3.01	60	88	141

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AB INITIO STUDY OF TRIATOMIC ALKALI HALIDES

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This contribution reports *ab initio* study of triatomic alkali halides. Excited rare gas atoms have similar ionization potentials and polarisabilities as alkali metal atoms. In turn this similarity lead to similarities between the ground state of MX molecules (M - alkali and X — halogen) and the ion-pair states of rare gas halide molecules (RgX). molecules. One may expect that the ground electronic state of triatomic M_2X molecules may have features in common with the bound $Rg_2X(4^2\Gamma)$ state of triatomic rare gas halides [1]. To compare properties of M_2X and Rg_2X molecules in a systematic way we performed calculations for all M_2X molecules containing Li, Na and K. Calculations for M_2^+ ions and MX were performed with the same method and basis sets as for M_2X molecules to obtain reference results for comparison. The M_2^+ and MX diatomics are well known from experimental and *ab initio* studies and the present results are in a good agreement with literature data. In contrast to the diatomics, M_2X molecules remain little studied. The results of the present work are summarized in Table 1. We note in particular that the bending mode frequency remain close to ν_e of $M_2^+(^2\Sigma_g)$ implying weak coupling with the symmetric stretch mode. Very similar result was obtained for Rg_2X molecules [1].

Table 1. Equilibrium internuclear distance (Å) and vibrational frequency (cm^{-1}) in the ground electronic state of M_2^+, MX, and M_2X molecules (M=Li, Na, K, X=F, Cl, Br, I). RASSCF/CASPT2 calculations with inclusion of the spin-orbit interaction, ano-rcc-v-qzp atomic natural orbital type basis set.

	M_2^+ $^2S^+_g$		MX $^1S^+$			M_2X 1^2A_1					
	$R_{M\text{-}M}$	v_e		$R_{M\text{-}X}$	v_e		$R_{M\text{-}X}$	$R_{M\text{-}M}$	v_a	v_s	v_b
Li_2^+	3.14	259	LiF	1.60	840	Li_2F	1.68	2.64	656	693	227
	3.14		LiCl	2.05	628	Li_2Cl	2.19	2.71		497	252
	3.14		LiBr	2.20	552	Li_2Br	2.35	2.73		439	243
	3.14		LiI	2.40	508	Li_2I	2.58	2.71		409	268
Na_2^+	3.61	122	NaF	1.97	475	Na_2F	2.03	3.17	400	365	118
	3.61	122	NaCl	2.38	354	Na_2Cl^a	2.53	3.22	206	281	119
	3.61	122	NaBr	2.52	294	Na_2Br	2.68	3.25	176	232	111
	3.61	122	NaI	2.71	258	Na_2I	2.89	3.27	156	207	111
K_2^+	4.50	74	KF	2.22	380	K_2F	2.30	3.95		284	70
	4.50	74	KCl	2.67	277	K_2Cl	2.83	4.06		213	69
	4.50	74	KBr	2.84	217	K_2Br	3.00	4.09	78	164	70
	4.50	74	KI	3.05	186	K_2I	3.24	4.12	108	142	62
^{a} literature results for Na_2Cl $R_{M\text{-}X}$=2.545 Å, $R_{M\text{-}M}$=3.263 Å, ref.[2]											

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CYCLOHEXANOL STRUCTURE AND IR SPECTRUM MODELING USING DENSITY FUNCTIONAL METHOD IN THE ANHARMONIC APPROXIMATION

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It was established that the cyclohexanol molecule has the property of conformational mobility. Cyclohexanol molecule is realized in the form of four conformers differ in the orientation of the hydroxyl group. By the method of neutron and X-ray diffraction analysis it was determined that the cyclohexanol is characterized by polymorphism, and forms the stable crystal structures with different molecular conformational composition. The structures of polymorphs is largely due to the influence of the hydrogen bonding. It was found that the crystalline phases II, III are formed by the endless chains, fragments of which are chained and cyclic tetramers respectively, and in an unstable phase III ‘ trimers are realized. All these H-complexes consist of cyclohexanol conformers with the equatorial orientation of hydroxyl group.

IR spectra of cyclohexanol were measured in the plastic (I) and crystalline (II, III) phases in a wide temperature range.

In this report we present the results of the simulation of the vibrational spectra of the isolated molecule of cyclohexanol in the anharmonic approximation. For calculation the selected model consisted of conformers, which more likely participate in the formation of H-complexes. The spectrum of cyclohexanol, calculated in the anharmonic approximation was compared with the spectrum calculated in the harmonic approximation using the procedure of frequencies scaling. In general, the spectra are the same, but the anharmonic frequencies of vibration involving hydrogen atoms are in better agreement with experiment. Accounting for mechanical anharmonicity in the calculation of the spectrum of cyclohexanol was improved the interpretation of the vibrational spectra.

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ЯДЕРНЫЙ МАГНИТНЫЙ РЕЗОНАНС И ЕГО ПРИМЕНЕНИЕ

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В современной физике термином «магнитный резонанс» называют совокупность явлений, возникающих при взаимодействии магнитных моментов ядер и электронов со статическими, переменными или флуктуирующими магнитными полями, которые либо прилагаются извне, либо могут возникать внутри вещества. Изменения ориентации магнитных моментов ядер или электронов в статическом магнитном поле сопровождаются излучением или поглощением квантов электромагнитного поля, соответствующему радиочастотному диапазону. Регистрируя это излучение и решая обратные задачи, можно извлечь информацию о локальной структуре молекул, различных твердых тел, о внутренних движениях в жидкостях, твердых телах, мезофазах и т.п. За развитие идей и приложений магнитного резонанса присуждено шесть Нобелевских премий по физике, химии, биологии, физиологии и медицине (последняя в 2003 году).

К магнитно-резонансным методам относятся в первую очередь:

- ядерный магнитный резонанс (ЯМР)
- электронный парамагнитный резонанс (ЭПР)
- ядерный квадрупольный резонанс (ЯКР)

Эти методы, являясь бесконтактными, не разрушают исследуемый объект, что делает их уникальными и востребованными не только в физике и химии, но и в медицине, геологии, биологии, археологии. В настоящее время ни один серьезный медицинский центр не обходится без ЯМР-томографа. В России ЯМР используется при каротаже нефтяных скважин, лабораторном анализе продуктивности нефтеносных коллекторов, анализе масличности и влажности семян, разработаны применения ЯКР для дистанционного обнаружения твердых взрывчатых и наркотических веществ, магнитометрические методы на основе магнитного резонанса незаменимы при проведении археологических изысканий.

ELEMENTAL PARTICLES OF DARK MATTER AND EXPERIMENTS ON ITS OBSERVATION

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The existence of dark matter in Universe is surely proved as a result astrophysical observations of star emission and also from theoretical predictions, obtained in high energy elemental particles physics [1,2]. To now in a number of theoretical and experimental works the nature of elemental particles of dark matter are thoroughly investigating. In this report the properties of such type particles are discussed. There are theoretical predictions, that the elemental particles of dark matter, named as paraphotons and axions [3,4], have very small rest mass: about 10^{-3} -1 meV, i.e, correspond to far infrared region of spectra. There are the "clouds" of slowly mowing of paraphotons and axions around of us and fast moving particles of dark matter from Sun or from cosmic space with velocity, close to c=3x10 m/s. The experiments on detection of paraphotons and axions in laboratory are described. In such experiments the modern lasers as the sources of exciting light for photon – paraphoton (axion) and some media as detectors for conversion processes realizing and detection have been used. The main property of elemental particles of dark matter is the opportunity of its propagation through the non-transparent media without any essential interaction. So the generation of directed beams of such type particles may be useful for space information transferring [5,6] and for another applications.

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ЕВОЛЮЦІЯ АКТИВНИХ ОБЛАСТЕЙ В КОРОНАЛЬНИХ ДІРКАХ

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Розглядається проблема існування активних областей (АО) у корональних дірках (КД). Існує думка, що КД є кінцевою фазою розвитку АО.

Було розглянуто повний цикл існування АО в КД. Були використані зображення Сонця в лінії HeI10830Å (Кр АО і в MLSO) і в лінії171 Å (SOHO). Я брав участь в отриманні зображень на БСТ-2, в їх обробці і роботі з архівами, з метою виявлення можливих випадків виникнення АО в КД. Були розглянуті спостереження за 1999–2005 роки і відібрано 5 випадків виникнення АО в КД. З архівів спостережень було отримано початкові файли, які згодом було унормовано до рівня спокійного Сонця.

Були проаналізовані зображення Сонця за весь час існування КД і АО в них, на різних рівнях атмосфери Сонця (хромосфера і корона). Після підрахунку площ КД на різних висотах було отримано відомості про висотну стратифікацію магнітного поля КД. У всіх випадках структура магнітного поля виявилася закритою.

КД, як правило, виникала не менш ніж за1оберт до появи в ній АО. Сама АО не змінювала розташування меж КД за весь час її існування, що особливо видно у двох випадках: коли АО з’являлася на межі КД або досягала її в процесі еволюції.

Після зникнення АО КД продовжувала існувати у своїх колишніх межах. Це свідчить про те, що КД є кінцевою фазою розвитку АО.

ДОСЛІДЖЕННЯ АСТЕРОЇДА 4 ВЕСТА

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У роботі розглянуті історія відкриття астероїда 4 Веста, фізичні характеристики астероїда за даними наземних спостережень та космічних апаратів. Описується АМС «Dawn» – дев'ята місія в рамках загального проекту Discovery Національної космічної агенції США (NASA), однією з цілей якої є вивчення астероїда 4 Веста.

Крім того, у роботі наводяться результати фотометричних спостережень астероїда, які були виконані у вересні 2012 року на 70-см рефлекторі Чугуївської спостережної станції Інституту астрономії ХНУ. Фотометрія була виконана за допомогою панорамного приймача випромінювання ПЗЗ-камери ML 47-10.

За результатами фотометрії була отримана його крива блиску у спектральних смугах BVRI, яка показала амплітуду $0{,}16^m$ при фазовому куті $23{,}15^o$. Крива блиску має відомий із літератури вигляд з одним широким максимумом і мінімумом за період обертання.Також була відмічена досить неочікувана особливість у поведінці колор індексів з обертанням астероїда.Отримані результати якісно узгоджуються з тими даними, що отримані з борту DAWN.

ДОСЛІДЖЕННЯ ТРАНЗИТУ ВЕНЕРИ ПО ДИСКУ СОНЦЯ

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Мета дослідження: вивчити і дослідити транзит Венери по диску Сонця, як рідкісне і унікальне астрономічне явище в Сонячній системі, яке спостерігається, коли планета в нижньому сполученні перетинає площину екліптики, зробити фотографії та проспостерігати транзит у часі, визначити відстань від Венери до Сонця, дослідити транзит Венери по диску Сонця за допомогою програми «Stellarium».

Актуальність:5-6 червня 2012 року люди востаннє у цьому столітті могли спостерігати транзит Венери по диску Сонця. Завдяки дослідженню транзиту Венери 2012 року було частково знайдено відповідь на питання про удосконалення методів дослідження атмосфер екзопланет. Ми мали рідкісну можливість особисто спостерігати в телескоп транзит Венери. Наступну таку можливість людство матиме аж в грудні 2117 року.

Завдання дослідження: здійснити спостереження транзиту 2012 року в місті Христинівка, вивчити історію досліджень шести транзитів, навчитись визначати відстані до планет, освоїти програму «Stellarium».

6 червня 2012 року з 5.00 до 7.54 год. було здійснено власне спостереження транзиту Венери.

При дослідженні транзиту Венери по диску Сонця 2012 року було зроблено світлини явища та помічено 7 плям на Сонці. За допомогою програми «Stellarium» було досліджено зміни відстані від Венери до Землі в момент нижнього сполучення. Також було досліджено транзит у часі, визначено відстань від Венери до Сонця (107080000 км=0,72 а.о.=$3{,}49 \cdot 10^{-6}$ пк) та визначено тривалість видимого транзиту 2012 року в різних містах світу і України.

ДОСЛІДЖЕННЯ ФОТОМЕТРИЧНОЇ ЗМІННОСТІ КАРЛИКОВОЇ НОВОЇ ТИПУ WZSGE OTJ184228

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Катаклізмічні змінні – це тісні подвійні системи, що знаходяться на пізніх стадіях еволюції. Вони складаються з компонента-донора – зірки пізнього спектрального класу, що втрачає свою речовину на компактний компонент – зірку, що знаходиться на пізній стадії еволюції.

Уявлення про процеси акреції дозволяють розібратися у фізиці більш екзотичних об’єктів: рентгенівських подвійних зірок, чорних дір та активних ядер галактик. Але найголовніше, що вивчення катаклізмічних змінних дозволяє всебічно поглянути на процеси еволюції зірок, що знаходяться на пізніх стадіях еволюції, в тому числі і на коричневі карлики.

Змінна OT J184228 була відкрита у вересні 2011 р. Через деякий час цей об’єкт спостерігали в обсерваторіях усього світу. Виявилося, що спалахова активність цієї зірки дуже примітна та не відповідає загальним особливостям спостереження таких змінних.

Автором проводилась обробка та аналіз знімків з 50-см телескопа ARCSAT, Apache Point Observatory, Нью-Мексико, США й отримання, обробка, аналіз знімків з 2,6-м телескопа ЗТШ, НДІ «Кримська астрофізична обсерваторія», с.Науковий, Україна.

Метою роботи є дослідження процесів, що протікають у карликовій нової OT J184228 під час згасання і після її надспалаху, методами сучасної астрофотометрії

За проведеними спостереженнями були відкриті пізні надгорби, та була виявлена короткоперіодична змінність з періодом, відмінним від орбітального. Також була розроблена фізична модель карликової нової, яка дозволяє пояснити усі фізичні процеси, які відбувалися в зірці.

ГРАВІТАЦІЙНЕ ЛІНЗУВАННЯ

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Луцька загальноосвітня школа І-ІІІ ступенів № 23 Волинської області, 10 клас,
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Гравітаційне лінзування – явище дуже “цікаве” для астрономів. Завдяки йому можна визначити багато невідомих величин: масу тіл, відстані до об’єктів, сталу Хаббла. Гравітаційним лінзам властива здатність збільшувати зображення, яскравість фонових об’єктів. Тому використання гравітаційного лінзування відіграє важливу роль серед методів дослідження космосу.

Об’єктом дослідження є гравітаційні лінзи, їх фізичні параметри, різновиди спотворених ними зображень, а також можливості Сонця, як гравітаційної лінзи.

Мета: збір та аналіз інформації про взаємодію світла і гравітаційного поля масивних тіл та вплив цього ефекту на видимі траєкторії небесних об’єктів. Відповідно до мети було поставлено такі **завдання:**

- розглянути історію дослідження гравітаційних лінз
- проаналізувати відомі знання про дане явище
- дослідити його вплив на видиме зображення космосу
- розглянути випадки спотворення зображень від фонових об’єктів при різних типах гравітаційних лінз
- дослідити використання даного явища вченими-астрономами для дослідження всесвіту
- обчислити параметри Сонця як гравітаційної лінзи.

Кожна зірка здатна бути гравітаційною лінзою, в тому числі і наше Сонце. Але, оскільки ми знаходимось близько до нього, то не можемо спостерігати цей ефект в повній мірі.

АНАЛІЗ ЗМІНИ КРИВОЇ БЛИСКУ ПОДВІЙНОЇ ЗОРІ WZ Crv

М.В. Могорян

Одеська Маріїнська гімназія, 10 клас,
Одеське територіальне відділення МАН

Подвійні зорі є основним джерелом інформації про маси зір,у подвійних зорях проходить багато фізичних процесів, які неможливо реалізувати у земних лабораторіях, тому вивчення таких зір є важливою задачею астрофізики.

Метою даної роботи було вивчення подвійної зорі WZ Ворона за допомогою аналізу ПЗЗ-зображень. Ставилася задача порівняти особливості кривої блиску цієї зорі 2012 року з більш ранніми спостереженнями, а також запропонувати пояснення феномену асиметрії кривої та дослідити його стабільність.

У 2010/2011 роках автор роботи розпочав дослідження подвійної зорі WZ Crv. Це затемнювана зоряна система типу Алголя з періодом 1.7887 днів. Автор відкрив у неї асиметрію максимумів блиску та повне затемнення у головному мінімумі. Результати цього дослідження опубліковані у статті Virnina N.A. Andronov I.L. Mogorean M.V. «A Hot Spotand Mass Transfer of the Algol-type Binary System WZ Crv».

У даній роботі представлено результати додаткових досліджень кривої блиску системи WZCrv за спостереженнями 2012 року, переобробленими спостереженнями 2010 року, та архівними спостереженнями електронних баз даних. У 2012 році спостереження велися у 4 фільтрах: *B*, *V*, *R*, *I*. На нових фазових кривих не помітно асиметрії, але головний мінімум помітно глибший, ніж був два роки тому. У роботі запропоновано пояснення феномену наявністю мігруючої «холодної» плями у фотосфері однієї з компонент та показано схематично її розташування у різні роки.

ЗІТКНЕННЯ В СОНЯЧНІЙ СИСТЕМІ: РОЛЬ І МЕТОДИ РОЗРАХУНКУ

Д.В. Шимків

Харківський навчально-виховний комплекс № 45 «Академічна гімназія»
Харківської міської ради Харківської області, 10 клас,
Комунальний заклад «Харківський центр дослідницько-експериментальної
діяльності «Будинок учителя» Харківської обласної ради»

Актуальність роботи базується на тому, що за останні два десятиліття була, не тільки усвідомлена серйозна небезпека для людства, пов'язана з падінням на Землю астероїдів і комет, але і здійснені активні дослідження різних аспектів цієї проблеми. Але це всього лише один із напрямків ще більш загальної задачі, що розглядає зіткнення в Сонячній системі будь-яких космічних тіл.

Метою роботи є стисло викласти основні аспекти цієї задачі (такі як астероїдна небезпека, роль зіткнень в еволюції Сонячної системи, а саме формування розподілу астероїдів за розмірами і формування рельєфу тіл, що володіють твердою поверхнею), висвітлити метод Епіка розрахунку ймовірності зіткнення. Було *поставлено завдання* проаналізувати основні положення методу Епіка, на прикладі конкретного потенційно-небезпечного астероїда показати можливості цього методу, написати програму та за її допомогою розрахувати для нього ймовірність зіткнення із Землею та порівняти отримане значення із результатами більш точних чисельних методів, перевірити чутливість результуючої ймовірності на зміну елементів орбіти ударника через збурюючий вплив планет та похибки астрометричних спостережень. При виконанні роботи був проведений аналіз літератури (переважно англомовної), описані якісні питання теорії зіткнень.

Зміст роботи включає два розділи. У першому наведені загальні відомості про малі тіла Сонячної системи, роль зіткнень у формуванні розподілу тіл за розмірами та на ранній стадії еволюції протопланетного диска, утворення кратерів на тілах Сонячної системи. Другий присвячений методу Епіка, оцінці впливу похибок у елементах орбіти на ймовірність зіткнення на прикладі астероїда (99942) Apophis з використанням оскулюючих елементів його орбіти на різні моменти часу. Написана програма, яка за елементами орбіти астероїда розраховує ймовірність його зіткнення із Землею.

Основні результати роботи: представлений метод розрахунку дозволяє швидко оцінити по порядку величини ймовірність зіткнення небесних тіл. Цю величину можна використовувати як верхню оцінку вірогідності зіткнення, а її обчислення істотно більш просте у порівнянні з точними, але громіздкими методами.

РОЗРОБКА ЕНЕРГОЗБЕРІГАЮЧИХ ТЕХНОЛОГІЙ ЕКСПЛУАТАЦІЇ ДЖЕРЕЛ СВІТЛА ШЛЯХОМ АНАЛІЗУ ЇХ СПЕКТРАЛЬНОГО ЕЛЕКТРОМАГНІТНОГО ВИПРОМІНЮВАННЯ

М.О. Козяр

Златопільська гімназія м. Новомиргорода Новомиргородської районної ради
Кіровоградської області, 10 клас,
Кіровоградське територіальне відділення МАН України

Актуальність теми. Економія електроенергії – це досить велика область реалізації раціональних намірів людини. Системи енергозбереження повинні забезпечувати високий ККД пристроїв на всіх етапах використання джерел енергії. Для штучних електричних джерел світла, в контексті впровадження енергозберігаючих інноваційних технологій, найважливішим є підвищення відсотка електричної енергії, яка безпосередньо трансформується в світлову, незалежно від типу джерела світла. Тому тема роботи є актуальною і відповідає сучасним тенденціям розвитку техніки.

Мета роботи – запропонувати технологію оптимізації технічних параметрів енергоефективної експлуатації джерел світла, шляхом аналізу відповідних спектрів електромагнітного випромінювання.

Завдання – вивчити теоретичні питання пов’язані з випромінювальними здібностями джерел світла та енергозберігаючими технологіями в даному напрямку, дослідити особливості оптичного спектру ламп, запропонувати технологію впровадження енергоефективного використання сучасних джерел світла.

Наукова новизна результатів –встановлено, що спектри випромінювання досліджуваних штучних джерел світла залежать від параметрів експлуатації при відхиленні від номінальних значень, а тому можливо в кожному окремому випадку встановлювати оптимальний режим їх роботи в контексті енергозбереження.

ДОСЛІДЖЕННЯ МОЖЛИВОСТЕЙ СТВОРЕННЯ ХВИЛЬОВИХ ЕЛЕКТРОСТАНЦІЙ ДЛЯ МОРСЬКИХ АКВАТОРІЙ УКРАЇНИ

А.П. Бурунін

Миколаївський морський ліцей імені професора М. Александрова
Миколаївської міської ради, 9 клас,
Миколаївське територіальне відділення МАН України

Енергія морського хвилювання нескінченна, отже хвильові електростанції (ХвЕС) – це альтернативні джерела екологічно чистої енергії, які є конкурентоспроможними серед інших джерел так званої «зеленої» енергетики.

Метою роботи є аналіз сучасного стану у галузі хвильової енергетики провідних морських країн світу, попередня оцінка доцільності розміщення ХвЕС на акваторії Азово-Чорноморського басейну України та експериментальне дослідження макету нового типу ХвЕС з гнучким енергопоглинаючими елементами.

Для досягнення поставленої мети у роботі вперше виконано огляд і порівняльний аналіз сучасних хвильових електростанцій та аналіз вод Азово-Чорноморського басейну України як джерел хвильової енергії, на підставі якого обрано перспективний для України тип ХвЕС з гнучкими енергопоглинаючими елементами. Запропоновано удосконалити механізм керування просторовим положенням ХвЕС з гнучкими енергопоглинаючими елементами по відношенню до напрямку набігання хвиль. Проведено басейновий експеримент. За результатами виконаних експериментальних досліджень макету ХвЕС встановлено залежності величини отримуваної механічної енергії на валу гнучкого елементу від довжини і ширини енергопоглинаючої стрічки і, таким чином, підтверджено працездатність ХвЕС нового типу.

ПРОГНОЗУВАННЯ КРИТИЧНОГО РУЙНУВАННЯ ЗРАЗКА ШЛЯХОМ ВИМІРЮВАННЯ ЙОГО ВЛАСНИХ ЧАСТОТ КОЛИВАНЬ

М.Д. Щедролосьєв

Херсонський фізико-технічний ліцей при Херсонському національному технічному
університеті та Дніпропетровському національному університеті, 10 клас,
Комунальний заклад «Мала академія наук» учнівської молоді
Херсонської обласної ради

У даній роботі нами представлений новий метод прогнозування критичних руйнувань – метод, оснований на вивченні вільних та вимушених коливань досліджуваної деталі. Цей метод ґрунтується на тому, щоб шляхом вимірювання власної частоти коливань резонансним методом можна було б спрогнозувати руйнування зразка.

Об'єктом нашого дослідження є вивчення міцнісних характеристик тіл.

Предметом нашого дослідження є вивчення зміни частоти коливань тіла у залежності від часу його експлуатації.

Завдання дослідження:

- з'ясувати механізм руйнування тіл, а також причини, що до цього призводять
- теоретично визначити залежність частоти коливань зразка від його міцнісних характеристик
- сконструювати установку для дослідження залежності частоти коливань зразка від кількості циклів навантаження та провести необхідні експерименти.

Причиною руйнування елементів конструкції в результаті появлення тріщин можуть бути корозія та старіння металу. Необґрунтоване продовження терміну експлуатації конструкції веде до різного роду аварій.

Нами встановлено теоретичну залежність частоти коливань досліджуваного зразка від його міцнісних характеристик.

Для підтвердження теоретичних результатів ми провели серію експериментів, спрямованих на вивчення залежності частоти коливань зразка від тривалості навантажень.

Нами розроблена установка, що піддає зразок циклічним навантаженням, розроблений спосіб визначення резонансної частоти коливань зразка для вивчення зміни його внутрішніх властивостей під дією циклічних навантажень.

Маючи графік залежності частоти від часу експлуатації або від кількості впливів на зразок, на якому чітко визначається, поблизу яких частот зразок руйнується, нам вдалося вибрати зразок з яскраво вираженою втомної характеристикою шляхом порівняння частот власних коливань зразка в справжній час з передкритичними частотами, зазначеними на графіку для серії однотипних екземплярів.

Теоретично та експериментально вдалося встановити, що в міру наростання втоми матеріалу змінюється модуль пружності, (Е - модуль Юнга), що веде до зміни швидкості поширення пружних хвиль і зміни власної частоти.

Надалі ми плануємо створити компактний і зручний прилад для здійснення подібних вимірів.

ВИГОТОВЛЕННЯ КРИСТАЛІВ ДЛЯ ОПТИЧНИХ ІЗОЛЯТОРІВ

Л.Я. Захарук

Чернівецький ліцей № 1 математичного та економічного профілів, 10 клас,
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Мета даної роботи — створення оптично досконалого для практичного використання напівмагнітного напівпровідника. Напівмагнітний напівпровідник Кадмій Манган Телур ($Cd_{1-x}Mn_xTe$) активно вивчається як перспективний представник твердих розчинів. Змінюючи процентний вміст компонентів ми можемо контрольовано впливати на властивості матеріалу. Наприклад, впливати на сталу Верде, змінюючи концентрацію магнітну компоненту Мангану.

Для вирішення поставленого завдання ми провели оптимізацію процесів вирощування монокристалів та дослідження питомого опору і спектра пропускання оптичного випромінювання кристалів $Cd_{1-x}Mn_xTe$ в залежності від вмісту Mn. Монокристали були вирощені у високотемпературних печах відповідно до модифікованого методу Бріджмена. Температурні режими печей були оптимізовані враховуючи фізичні і хімічні властивості твердих розчинів і результати досліджень. Процес проходив у кварцових контейнерах, покритих піролітичним графітом. Для синтезу були застосовані ультра-чисті компоненти. Це дало можливість запобігти оптичному поглинанню домішками в області енергії фотонів, що менше, ніж ширина забороненої зони. Вміст марганцю було змінено в різних кристалах з x=0,04, x= 0,5.

Така робота є актуальною завдяки перспективності і попиту на такий прилад як оптичний ізолятор. Нашою метою було отримати кристали $Cd_{1-x}Mn_xTe$, які би підходили для практичного використання, і дослідити їх властивості. Ми оптимізували і модифікували процес росту кристалу і дослідили спектральну залежність оптичного пропускання кристалу $Cd_{1-x}Mn_xTe$ залежно від вмісту Мангану.

КЛАСИЧНІ ТА РЕЛЯТИВІСТСЬКІ ОСОБЛИВОСТІ ОПИСУ РУХУ ТІЛ У ПРИРОДНИХ КООРДИНАТАХ

М.С. Дмитрієв

Комунальний заклад освіти «Дніпропетровський ліцей інформаційних технологій
при Дніпропетровському національному університеті імені Олеся Гончара», 10клас,
Комунальний позашкільний навчальний заклад
«Мала академія наук учнівської молоді» Дніпропетровської обласної ради

В роботі розглядаються геометричні конструкції, які зустрічаються у курсу фізики.Особливо детально вивчено опис траєкторій та законів руху тіл під дією центрального поля тяжіння.Зміна параметризації у такому русі тіл дозволяє оперувати поняттями кривини.Розглядаються випадки, коли кривину траєкторії тіла можна вважати сталою, а також для еліптичного руху у полі тяжіння.Розглянуті також випадки коли крім кривини є ще один параметр - кручення.Як приклад, розглядається рух заряджених частинок (електронів) біля полюсів Землі у її магнітному та гравітаційному полях.

Введення полярних координат, функцій кривини траєкторії від довжини траєкторії (k=k(l)). Опис руху через полярні, природні координати та використання градієнту гравітаційного поля.

Опис та параметризація траєкторій тіл як кривих ліній, що належать одній площині, у викривленому гравітаційним полем просторі. Розв’язок з динамічної та енергетичної точок зору за сталої кривини траєкторії.Розглянуті аналогії та зв’язки зі спеціальною та загальною теорією відносності.

ДОСЛІДЖЕННЯ ТЕМПЕРАТУРНИХ ПОЛІВ ВОДНОГО СЕРЕДОВИЩА (НА ПРИКЛАДІ РІЧКИ КОЛОМАК)

Г.О. Канцедал

Полтавський обласний ліцей-інтернат для обдарованих дітей із сільської місцевості
ім. А.С.Макаренка, 9 клас,
Позашкільний навчальний заклад Полтавської обласної ради
«Полтавська обласна Мала академія наук учнівської молоді»

За останні роки накопичено багато дослідного матеріалу, який змінює підходи спеціалістів до розуміння процесів, які відбуваються в гідросфері. Практична направленість дослідження різних форм води, що полягає у вивченні антропогенних впливів на водні екосистеми у XXI столітті, стає **актуальною**. Це диктує необхідність детального фізичного і математичного опису властивостей і процесів, що проходять в водному середовищі, великих і малих річках країни.

Мета роботи – розглянути особливості зміни температури водоймища з врахуванням факторів, які приводять до зміни температури води в річці та запропонувати модель явища, яка адекватно описує температурні поля річки в різні пори року, що розв’язується в рамках підходу гідрофізики.

Досягнення поставленої мети передбачає розглянути стан досліджуваної проблеми в сучасній фізичній теорії, аргументувати доцільність використання запропонованої фізичної моделі зміни температурних полів річки Коломак, провести експериментальні дослідження температури водного середовища і побудувати модель зміни температури водоймища від впливу теплових потоків та розкрити особливості фазових та циклічних змін температури з часом.

У роботі зроблена спроба описати вплив фізичних факторів на температурні поля річки Коломак, які ґрунтуються на врахуванні фізичних властивостей води.

Отримані результати можуть бути використані при вивченні особливостей фізичних процесів, які протікають в водоймищах в рамках гідрофізики, що враховує такі фізичні процеси як випаровування в природних умовах, нагрівання і охолодження водоймищ, утворення і зникнення льодяного покриву, течій.

МОДЕЛЮВАННЯ РУХУ ЕЛЕКТРИЧНИХ ЗАРЯДІВ В ЕЛЕКТРИЧНИХ ТА МАГНІТНИХ ПОЛЯХ

О.Г. Челпанова

Херсонський фізико-технічний ліцей при Херсонському національному технічному
університеті та Дніпропетровському національному університеті, 10 клас,
Комунальний заклад «Мала академія наук» учнівської молоді
Херсонської обласної ради

Робота присвячена аналізу руху електричних зарядів в електричних та магнітних полях за різних значень початкових параметрів.

На основі аналізу законів руху зарядів у електричних та магнітних полях отримані рівняння залежності координат зарядів від часу, які покладені в основу побудованих моделей. У роботі детально описуються траєкторії руху електричних зарядів у постійних та змінних електричних та магнітних полях в залежності від початкових умов.

На основі одержаних рівнянь у тривимірному просторі за допомогою СКМ MATLAB побудовано відповідні графіки траєкторій руху зарядів, проаналізовані їх відмінності.

ПРИНЦИПИ СУЧАСНОГО БЕЗДРОТОВОГО ЗВ'ЯЗКУ

Р.В. Моцар

Сагайдацька загальноосвітня школа I-III ступенів Шишацької районної ради
Полтавської області, 10 клас,
Позашкільний навчальний заклад Полтавської обласної ради
«Полтавська обласна Мала академія наук учнівської молоді»

Серед відмінних якостей безпровідних технологій найбільш очевидною є їх мобільність. Це надає безпровідним мережам суттєвої переваги. Однак, принциповим недоліком залишається складність з'єднання рухомих абонентів.

Сфера використання бездротового Інтернету розширюється, зростає і число його користувачів та пристроїв для швидкого виходу до нього. Тому **актуальним** є і наше дослідження.

Мета роботи:

- ознайомитися з фізичною суттю бездротового зв'язку
- вивчити структуру та принцип роботи сучасного безпровідного зв'язку
- виявити зміну поколінь і стандартів
- вивчити технічні параметри та принцип роботи мережі Wi-Fi
- провести дослідження залежності швидкості з'єднання від відстані, наявності перешкод та кількості користувачів
- виявити переваги і недоліки мережі Wi-Fi.

Завдання роботи:

- вивчити теоретичний і довідковий матеріал з теми
- вивчити сучасний стан та перспективи розвитку безпровідних мереж
- провести налаштування безпровідної мережі Wi-Fi та дослідити її.

Основними результатами роботи є: створення алгоритму для налагодження мережі в умовах закритого приміщення, проведенні теоретичних досліджень, тестуванні мережі та узагальненні даних та написанні наукової роботи.

Практичне значення полягає у систематизації та використанні результатів роботи при проведенні факультативних занять та профільному вивченні принципів сучасного безпровідного зв'язку.

ПРИРОДА ВПЛИВУ МАГНІТНИХ БУР НА ОРГАНІЗМ ЛЮДИНИ

О.А. Терентьєв

Роменська спеціалізована загальноосвітня школа І-ІІІ ступенів № 1
ім. П.І. Калнишевського Сумської області, 10 клас,
Сумське територіальне відділення МАН України

Магнітне поле Землі є однією із захисних оболонок всього живого на ній.

В результаті підвищеної сонячної активності величезні потоки сонячного вітру, який складається із потоку ультрафіолетової, рентгенівської та інших типів радіації, потоку корпускулярних частинок, виникають магнітні бурі, які стають причиною погіршення самопочуття деякої категорії людей з хронічними захворюваннями.

Отже, **предметом наших досліджень** є вивчення впливу вихрових магнітних бур на живі організми, та зокрема на організм людини.Пояснення фізичної природи зміни самопочуття людей під час даних магнітних аномалій.

Оскільки нам відома зовнішня причина цих ускладнень, то ми можемо допустити, що причиною самих ускладнень є гістерезис провідності деяких структур у складі живого організму, зокрема людини (наприклад клітинних мембран, різноманітних розчинів в середині організму). Перевірка правильності цього допущення і є **метою** цієї роботи.

Спочатку, розкриємо суть проблеми у теоретичній частині, висвітливши питання магнітних явищ, та провідності.

Щоб підтвердити запропоновану теорію проведемо серію експерементів над речовинами, які містяться в організмі людини або схожі з ними за властивостями.Саме тому ми обрали питну воду (адже в організмі людини води в чистому вигляді немає), розчин кухонної солі, медичний розчин NaCl, розчин рідкого мила (аналог рідких кристалів, які являють собою мембрани клітин людського організму), глюкозу.Також проведемо серію дослідів над медичними препаратами рибоксином та магнезією.

Перший блок включає в себе речовини, опір яких вимірювався не постійно, а методом багаторазових замірювань.Другий блок включає речовини, опір яких вимірювався постійно, так як вони постійно знаходились у електричному колі.

Можемо зробити висновок, що на такі речовини як вода, кухонна сіль, рибоксин та магнезія магнітне поле не впливає взагалі. На розчин NaCl характер та міру впливу важко встановити, так як проведений дослід не вдалося повторно відновити.На такі речовини, як кров, рідке мило, глюкозу певний вплив однозначно є.

ДОСЛІДЖЕННЯ ВЛАСТИВОСТЕЙ ТЕЧІЙ СИПКИХ СЕРЕДОВИЩ

С.І. Маринін

Тернопільська спеціалізована школа I-III ступенів № 5
з поглибленим вивченням іноземних мов, 10клас,
Тернопільське обласне комунальне відділення МАН України

В роботі проведено дослідження потоку сипкої речовини (сухого кварцового піску). Ряд проведених експериментів та обробка їх даних засвідчили, що коефіцієнт опору середовища при обтіканні ним циліндричного тіла сталих розмірів залежить від швидкості. Було побудовано графік залежності цього коефіцієнта***k*** від швидкості руху циліндра в піску. Всі дослідження будувалися на відомій, але мало розвинутій думці, що сипке середовище за певних умов може поводити себе як неньютонівська рідина.Згідно цього твердження була побудована відповідна модель обтікання потоком сипкого середовища циліндричного тіла за умов, коли сипкий матеріал можна моделювати неньютонівською рідиною.

Результати проведених досліджень планується використати у подальшому вивченні властивостей течій сипких середовищ і побудови залежності коефіцієнта внутрішнього тертя сипкого середовища від швидкості руху досліджуваного тіла.

МОНІТОРИНГ ШУМОВОГО ЗАБРУДНЕННЯ

Т.В. Шевчук

Комунальний заклад «Луцький навчально-виховний комплекс №26»
Волинської області, 10 клас,
Комунальна установа «Волинська обласна Мала академія наук»

На сьогодні, в умовах зростаючої психоемоційної напруженості та інтелектуалізації трудових процесів навіть низькі шуми викликають додаткові навантаження на організм людини. Це зумовило **актуальність** вибору теми дослідження.

Мета роботи : моніторинг шумового забруднення школи, мікрорайону школи, прилеглих територій (проспекту Соборності) та визначення залежності між рівнем шуму і здоров’ям людини.

Завдання дослідження:

- провести бібліографічний огляд літератури з вибраної тематики
- проаналізувати, систематизувати та вивчити отриманий матеріал
- розробити програму яка б дозволяла визначати рівень звуку (затухання хвилі),
- визначити метод дослідження вимірювання рівня шуму
- ознайомитись з будовою приладу для проведення шумометрії та навчитись ним користуватись
- вибрати відповідні місця та режими проведення моніторингу
- провести моніторинг шумового забруднення школи, мікрорайону школи, прилеглих територій (проспекту Соборності)
- визначити залежності між рівнем шуму і здоров’ям людини
- розробити поради щодо зменшення шуму
- сформулювати відповідні висновки.

Проведений моніторинг виявив, що рівень шуму у школі перевищує санітарну норму на 15–20 дБ.

ДИФРАКЦІЯ РЕНТГЕНІВСЬКИХ ПРОМЕНІВ НА КРИСТАЛАХ

А.І. Замковська

Загальноосвітня школа І-ІІІ ступенів № 18 Сімферопольської міської ради
Автономної Республіки Крим, 10 клас,
Республіканський позашкільний навчальний заклад «Мала академія наук учнівської молоді Автономної Республіки Крим «Шукач»

Мета роботи: вивчити теорію дифракції рентгенівських променів на кристалах.

Об’єкт дослідження: кристалічна структура невідомих кримських мінералів.

Методи дослідження, апаратура: метод рентгеноструктурного аналізу (РСА), дифрактометр загального призначення (ДРОН-3).

Актуальність роботи: метод рентгеноструктурного аналізу є основним методом визначення природи кристалічних речовин.

Завдання роботи:

- Ознайомитись з теоретичними основами методу РСА
- Застосувати цей метод до дослідження кристалів
- Представлена робота присвячена сторіччю досліду М. Лауе по дифракції рентгенівських променів на кристалах. Метод рентгеноструктурного аналізу є унікальним методом встановлення природи кристалічної речовини і його структурних характеристик за допомогою рентгенівських променів.

Методом РСА була вивчена кристалічна структура двох невідомих зразків кримських мінералів.

Висновок: досліджувані мінерали є кварцами. Прозорий зразок - гірський кришталь. Непрозорий зразок - молочний кварц.

ОЛІВЕЦЬ-МАНДРІВНИК

А.А. Распутько

Донецька спеціалізована фізико-математична школа № 17, 10 клас,
Донецьке територіальне відділення МАН

У своїй роботі я досліджував поведінку грифеля олівця при його падінні. При цьому початкове положення олівця було перпендикулярно поверхні, по якій ковзав його грифель.

Мене зацікавила ця робота, тому що мені подобається спостерігати за простими речами і намагатися пояснити їх з погляду законів фізики.

На підставі простої якісної моделі я зрозумів, що спочатку падіння олівець завжди прагне зсунутися проти напряму падіння. Якщо тертя велике, то воно його утримує від такого руху. Якщо маленьке, то олівець починає ковзати проти напряму падіння. В другій половині олівець завжди прагне ковзати у напрямі падіння. Тому, за незначного тертя він, врешті-решт, хоч трохи ковзає в цей бік. Зроблений висновок я потім підтвердив і теоретично й експериментально.

У своїй роботі я розробив теоретичну модель, що дозволяє розраховувати рух олівця при падінні і визначати напрям зсуву грифеля залежно від умов тертя.

Експериментальна перевірка показала, що теоретична модель добре передбачає реальну поведінку олівця. Проте є деяка розбіжність даних, пов’язана, на мою думку, з тим, що фактичне переміщення грифеля олівця залежить не тільки від коефіцієнта тертя, але і від форми заточування грифеля, сили притиску при установці олівця в початкове положення, напрямку падіння тощо.

При заміні звичайного паперу наждачним, коефіцієнт тертя зростає у багато разів, і грифелі всіх олівців ковзають у напрямку падіння олівця.

При сильному зменшенні коефіцієнта тертя (заміна звичайного паперу на дуже гладку, слизьку поверхню столу) грифелі всіх олівців спочатку ковзають назад.

ПРОХОДЖЕННЯ «БОГИНІ КОХАННЯ» ПО ДИСКУ СОНЦЯ

О.О. Сенченко

Загальноосвітня школа I-III ступенів № 8 Вінницької міської ради, 10 клас,
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6 червня 2012 року весь світ захоплено спостерігав за неймовірним явищем – проходженням Венери по диску Сонця. Це астрономічне явище спостерігається коли планета Венера, під час свого орбітального руху, опиняється на лінії між Землею та Сонцем. Таким чином, диск Венери проектується на диск Сонця й, відповідно, частково затемняє невелику ділянку сонячного диску, світло від якої не доходить до земного спостерігача.

Саме в той час, коли Венера сягає точки внутрішнього сполучення, або перебуває поблизу неї, може спостерігатися явище транзиту Венери. Загалом послідовність транзитів повторюється кожні 243 роки. Вона складається з двох пар явищ (два сусідні транзити розмежовані між собою в часі на вісім років), які відбуваються пара за парою через 121,5 рік та 105,5 роки.

Ефект «чорної краплі» («чорного падіння») - видима розмитість краю Венери по відношенню до краю Сонця під час проходження Венери по його диску.

Явище проходження Венери по диску Сонця викликає підвищений науковий інтерес. Це й не дивно, адже за допомогою даних, отриманих під час спостережень транзиту, можна:

- обчислити значення сонячного паралакса,
- розрахувати відстань Земля-Сонце,
- визначити розміри Сонячної системи,
- використати цей метод при знаходженні екзопланет.

Саме під час транзиту Венери по диску Сонця у 1761році М. В. Ломоносов виявив, що на ній існує атмосфера.

З того часу, як людство вперше спостерігало проходження Венери по диску Сонця, зроблено багато відкриттів: з’явилися нові технології, відкрито нові закони, виміряні відстані до космічних тіл, визначені константи.

Не змінним залишається одне – цікавість людства до цього явища, яка не згасає, а тільки розгорається все новими і новими питаннями та можливостями.

ПРИЛАД ДЛЯ ЛАБОРАТОРНИХ РОБІТ З ДОСЛІДЖЕННЯ МАГНІТНОГО ПОЛЯ ПОСТІЙНОГО МАГНІТУ

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Основною метою роботи є створення приладу, який дозволяє дослідити магнітне поле постійного магніту.

Для розв’язання задачі ми розробили прилад, за допомогою якого можна досліджувати магнітне поле в лабораторних умовах. Пристрій дозволяє виміряти індукцію магнітного поля. Для проведення дослідження потрібні джерело живлення (акумулятор., лабораторний амперметр, ключ замикання струму, реостат лабораторний магніт та прилад для вимірювання індукції магнітного поля. Див рис.1

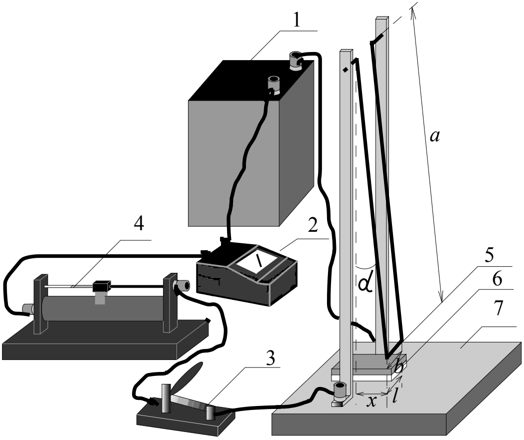

Рис. 1 Прилад для дослідження магнітного поля

1. джерело живлення (акумулятор. 2. амперметр лабораторний, 3. ключ замикання струму, 4. реостат лабораторний, 5. провідник, що знаходиться в магнітному полі, 6. постійний магніт, 7. прилад для вимірювання індукції магнітного поля постійного магніту.

Теоретичний аналіз проблеми та проведені нами експерименти дозволили розробити лабораторну роботи виконання якої дозволить кількісно і якісно дослідити поле постійного магніту.

ДОСЛІДЖЕННЯ БУДОВИ ПОЛІМЕРНОГО МАТЕРІАЛУ ПЛАЗМОХІМІЧНОЇ ГІДРОФОБІЗАЦІЇ АМІАЧНОЇ СЕЛІТРИ ЗА ДОПОМОГОЮ ІНФРАЧЕРВОНОЇ СПЕКТРОСКОПІЇ

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Актуальною стає розробка нових технологій формування тонкоплівкових полімерних покриттів на поверхні твердих тіл і надання матеріалам особливих властивостей шляхом використання інфрачервоної спектроскопії для дослідження будови полімерного покриття.

Об’єкт досліджень - в роботі висвітлено питання використання низькотемпературної плазми для гідрофобізації дисперсних неорганічних речовин.

Предмет досліджень - кондиціювання мінеральних добрив на прикладі аміачної селітри шляхом нанесення на поверхню гранульованого добрива полімерної плівки заданої товщини, будови і властивостей із застосуванням інфрачервоної спектроскопії для встановлення механізму одержання матеріалу покриття гранул із газової фази низькотемпературної плазми органічної речовини.

Мета досліджень - ліквідація злежуваності нітрату амонію NH_4NO_3, зменшення швидкості розчинення аміачної селітри в контакті з вологою, збільшення коефіцієнту використання рослинами сільськогосподарських культур аміачної і нітратної форм азоту та ліквідації забруднення ґрунтових, річкових і озерних вод нітратами, що має **практичне значення** як для промислового виробництва цього та інших видів добрив. Це дає можливість зберігання і транспортування партій добрив значних об’ємів без втрати їх фізико-хімічних та фізико-механічних властивостей. Запропонований спосіб капсулювання будь-якого гранульованого мінерального добрива або покриття зерен дисперсного матеріалу гідрофобною плівкою надає їм нових властивостей і в цьому **новизна роботи**.

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LAST MINUTE ABSTRACTS

RADIO EMISSION OF NANOPARTICLES IN THE COMBUSTION PRODUCTS PLASMA OF SOLID ROCKET FUELS

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Radio-frequency component of electro-magnetic radiation (EMR) of plasma-dusty formations (PDF), in rarefied atmosphere or cosmic space, appears as a result of complex interaction between structural PDF elements and self- self consistent electro-magnetic field of the system. Generation of long-wave radiation by plasma medium is created, first, by the slowing-down radiation of charges which acquire acceleration in a self-consistent electrostatic field of the system. Due to that it, radio-component EMR carries in itself integrated information concerning the motion and interaction of PDF charges. For non-relativistic speeds of charged PDF particles of the magnetic component of the charge interaction it is possible to disregard, so the problem of describing EMR characteristics of the plasma system can be limited to, describing the motion of plasma free charges in the electrostatic field, which they create jointly, coordinating their motion in the phase space due to correlations. Because of the far-reaching action of coulomb forces, solving the problem of micro fields and charges interaction in plasma medium meets classical complication of the theory of many bodies with long-range Coulomb interactions far-acting power, i.e. the impossibility of bringing potential energy of structural elements (the charges of the system) down to pair interaction. Using continual statistic approach, based on the definition of density functional of the potential energy of PDF gives the possibility to bring the problem down to an effective electrostatic problem, but also demands the elaboration of new methods of statistic equation for parameters of the system with far reaching coulomb far action [1-3].

In the paper, we use a method of statistical equation (averaging) of the charge density according to the ensemble of the “electroneutral cells in plasma” and the definition of effective distribution of local electrostatic potential in heterogeneous plasma medium. The evolution of location and motion of separate charges is viewed as a temporary sequence of their anharmonic oscillations in the excited cell of electrical neutrally PDF, in which distribution of the local electrostatic field "is checking" "to keep track of" activated displacement of a separate charge from equilibrium position. Results of computer simulation to define spectral components of plasma radiation of the products of powdered aluminum combustion in the atmosphere air were compared to the data of natural experiments. Very good qualitative and quantitative coordination of the data of both the computer and the natural experiments were observed.

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