XX International School-Seminar of Galyna Puchkovska

SPECTROSCOPY OF MOLECULES AND CRYSTALS

Book of Abstracts

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CONTENT

THE FOUNDING OF GALYNA PUCHKOVSKA INTERNATIONAL SCHOOL-SEMINAR "SPECTROSCOPY OF MOLECULES AND CRYSTALS"

The International School-Seminar "Spectroscopy of Molecules and Crystals" named after Professor Galyna Puchkovska is the result of a lengthy and exciting history. Its development began in 1973, and was initiated by a working group in the Institute of Physics, Kyiv, Ukraine; it concluded with the organization of the Ist School-Seminar by its two architects: the Chairman, then director of the Institute of Physics, Member of the National Academy of Sciences of Ukraine Marat Shpak, and the Secretary, then senior researcher in the department of infrared spectroscopy, later a Head of Photoactivity Department, professor Galyna Puchkovska, who became the heart and soul of the school from the start. Among the founders of the School-seminar was also its Honorary Chairman since 1979, world-known physisist and theoretician, Member of the National Academy of Sciences of Ukraine Alexander Davydov.

Galyna Puchkovska had always taken an interest in seemingly distant scientific fields and therefore enjoyed the opportunity for a lively exchange of ideas with colleagues. The key to this approach had been handed to her in her early years by her parents and elder sister, who had taught her to respect people of different views and philosophies, and to seek dialogue with specialists working in different field of research. Since the very beginning, the topics of the school-seminar include theoretical spectroscopy, molecular dymanics and molecular interactions, spectroscopy of molecular crystals, spectroscopy of inorganic crystals and semiconductors, as well as instruments and methods of spectroscopy.

With her vision of a school-seminar, Galyna Puchkovska aimed at a clearly-defined goal: with the help of wide-cirle meetings of scientists and engineers, the problems and questions of molecular spectroscopy and its applications should be

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examined from different perspectives. Since the very beginning, the School-Seminar has become regular meetings of prominent scientists from all-around the former USSR held in different locations throughout Ukraine.

The Ist School-Seminar was held in the Western Ukraine near Uzhorod at the sport and recreation camp "Skalka"of Uzhgorod University, and was attended by about 80 participants from Ukraine, Russia, Bielorus and other former Soviet countries. Among the lecturers of the First school-seminar were such famous scientists, as world-known great Russian physisit Member of the Academy of Sciences of USSR since 1939 year V.A. Fok (Moscow), Member of the National Academy of Sciences of Ukraine M.P. Lysytsa (Kyiv), Member of the Russian Academy of Sciences Yu.I. Pentin (Moscow), professor A.V. Iogansen (Moscow), professor V.M. Zolotarev (St.-Petersburg). The first school-seminar was very successful, and at its closing ceremony it was decided to held it every two years. To a large extend, the great success of the school-seminar, as well as its future big popularity, was based on extremely warm and friendly atmosphere which was always characteristic for Galyna Puchkovska's personality. Apart from very exciting scientific programme, the participants of the First school-seminar remember its interesting cultural programme, including excursion to Nevitsky Castle, walking tour over Carpathian mountain medows, discussions near bonfire with guitar songs, as well as hot sport battles. Among the architechts of Galyna Puchkovska School-seminar, who remained its great devotees for long years, were now widely-known famous scientists from former USSR, such as professors Ye.M. Aver'yanov (Krasnoyarsk), L.M. Babkov (Saratov), L.M. Blinov (Moscow), S.S. Bukalov (Moscow), S.F. Burejko (St.-Petersburg), O.V. Ch-

alyi (Kyiv), Yu. Gaididej (Kyiv), Corresponding Member of the Russian Academy of Sciences L.A. Gribov (Moscow), professors O.P. Demchenko (Kyiv), A. Djumabaev (Samarkand), I.P. Ipatova (St.-Petersburg), V.O. Khranovskii (Kyiv), L. Kimtis (Vilnius), N.I. Koroteyev (Moscow), P.A. Korotkov (Kyiv), L.A Leites (Moscow), N.D. Orlova (St.-Petersburg), Member of the Russian Academy of Sciences Yu.A. Pentin (Moscow), professors Yu.N. Panchenko (Moscow), Yu.N. Polivanov (Moscow), V.Ye. Pogorelov (Kyiv), Ye.V. Ryl`tsev (Kyiv), A.V. Sechkarev (St.-Petersburg), Corresponding member of the National Academy of Sciences of Ukraine V.Yo. Sugakov (Kyiv), Doctor of Science A.Ye. Semenov (Kemerovo), professor E.N. Myasnikov (Rostov-on-Don), Member of the Russian Academy of Sciences V.B. Timofeev (Chernogolovka), Member of the Russian Academy of Sciences V.F. Shabanov (Krasnoyarsk), Corresponding Member of the National Academy of Sciences of Ukraine M.Ya. Valakh (Kyiv), Corresponding Member of the Russian Academy of Sciences Ye.A. Vinogradov (Troitsk), professors G.N. Zhizhin (Moscow), P.M .Zorky (Moscow), Member of the Academy of Sciences of Bielorus R.G. Zhbankov (Minsk).

Galyna Puchkovska also held the opinion that the School-Seminar should be the means to exchange an experience and to facilitate joint research in different fields of spectroscopy. With time, the popularity of the School-seminar grown and the number of its participants widen. Some additional scientific sections were added to its topics, such as spectroscopy of liquid crystals (headed by professor Yu. Reznikov), spectroscopy of biological objects and biopolymers (headed by corresponding member of the National Academy of Sciences D.M. Govorun), as well as laser spectroscopy and non-linear optics (headed by corresponding member of the National Academy of Sciences of Ukraine M.Ya. Valakh). This allowed to involve for particiaption in the school-seminar even wider circles of skilled professionals and scientific youth from the most up-to-date fields of science and technology.

Since 1991, (after the disintegration of former Soviet Union) the School-Seminar turned into an international meeting. The First Interational (Xth) School-Seminar of Galyna Puchkovska was held in Klementove village (at a recreation center "Electron" of Sumy Electronic Microscope Plant) with participation of scientists from the former Soviet Union and European countries. First European participants of the school-seminar were scientists from Poland — Member of Polish Academy of Sciences professor Henryk Ratajczak, professors Zdislaw Latajka and Grazina Bator, and Slovenia — Dr. R. Jerman. In the following years, the school-seminar was attended by a number of prominent world-known scienticsts, among them professor C. Sandorfy (Canada), professor S. Bratos (France), member of Polish Academy of Sciences professor L. Sobczyk (Poland), profes-

A group of participants of VI SSSMC (Chernigiv, 1983) on sightseeing tour over Desna river

sors A. Koll (Poland), M. Szafran (Poland), S. Dega-Szafran (Poland), G. Lashenal (France), S. Turrell (France), B. Engelen (Germany), M. Shattke (Germany), M. Zaworotko (USA), S. Suto (Japan), and most of them were also the competent members of International Advisory Board of the School-seminar.

The geography of the School-Seminar covers nearly all famous places of Ukraine:

I SSSMC — Uzhgorod (1973)
II SSSMC — Lutsk (1975)
III SSSMC — Mukacheve (1977)
IV SSSMC — Chernivtsi (1979)
V SSSMC — Cherkasy (1981)
VI SSSMC — Chernigiv (1983)
VII SSSMC — Odessa (1985)
VIII SSSMC — Poltava (1987)
IX SSSMC — Ternopil (1989)
X ISSSMC — Sumy (Klementove) (1991)
XI ISSSMC — Kharkiv (1993) — dedicated to the memory of the Member of the Academy of Sciences of the USSR A.S. Davydov
XII ISSSMC — Nizhin (1995) — dedicated to the memory of the Member of the Academy of Sciences of the USSR M.T. Shpak
XIII ISSSMC — Sumy (1997)

XIV ISSSMC — Odessa (1999)
XV ISSSMC — Chernigiv (2001)
XVI ISSSMC — Sevastopol (2003)
XVII ISSSMC — Beregove, Crimea (2005)
XVIII ISSSMC — Beregove, Crimea (2007)
XIX ISSSMC — Beregove, Crimea (2009)
XX ISSSMC — Beregove, Crimea (2011) — ANNIVERSARY!!!!

Galyna Puchkovska had always sought for possibilities to support young Ukrainian researches. She realized that the international meetings such as the School-Seminar may help them to present their ideas before international spectroscopic community and to initiate common research projects with European scientists and engineers. Every year, the School-Seminar widens the number of its participants, and 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 Ukraine, Russia, Belorus, Armenia, Uzbekiston, Latvia, Luthuania, and other countries. An important part in the organization of the school-seminars in different years took V.V. Artamonov (Kyiv), O.I. Barabash (Kyiv), T.V. Bezrodna (Kyiv), I.V. Blonsky (Kyiv), I.Ye. Boldeskul (Kyiv), G.I. Gaid-

Some statistical data on Galyna Puchkovska International School-Seminar "Spectroscopy of Molecules and Crystals"

Event date and location	General number of participants	Number of Professors (Doctors of Sciences)	Number of Doctors (Candidates of Scineces)	Number of participating countries
1973 (Uzhgorod)	83	3	26	—
1975 (Lutsk)	140	8	65	—
1979 (Chernivtsi)	250	18	112	—
1987 (Poltava)	206	36	125	—
1989 (Ternopil)	201	28	107	—
1991 (Sumy-Klementovo)	97	17	38	8
1995 (Nizhin)	105	20	33	6
1999 (Odesa)	102	33	45	14
2001 (Chernigiv)	109	30	44	8
2003 (Sevastopol)	135	44	69	10
2005 (Beregove)	170	40	54	7
2007 (Beregove)	177	37	50	9
2009 (Beregove)	136	36	43	4

idej (Kyiv), T.A. Gavrilko (Kyiv), N.A. Golovina (Lutsk), V.V. Gotsulsky (Odessa), N.A. Davydova (Kyiv), N.L. Dmitruk (Kyiv), G.V. Klimusheva (Kyiv), S.I. Kshnyakina (Sumy), V.V. Koronin (Kyiv), S.P. Makarenko (Kyiv), Yu. Levchuk (Kyiv), O.V. Lizengevich (Kyiv), T.V. Lokotosh (Odessa), M.P. Malomuzh (Odessa), V.I. Melnyk (Kyiv), S.G. Nedilko (Kyiv), L.V. Poperenko (Kyiv), V.Yu. Reshetnyak (Kyiv), Yu.O. Reznikov (Kyiv), V.M. Rozenbaum (Kyiv), V.Ya. Reznichenko (Kyiv), S.O. Samijlenko (Kyiv), T.I. Semenets (Kyiv), I.V. Sekirin (Kyiv) and many-many others.

Since 2005, organization of Galyna Puchkovska School-Seminar was handed over to Taras Shevchenko National University of Kyiv with its sport and recreation center in Beregove village of Crimea, where the School-seminar found its permanent residence. The Organizing Committee of the School-Seminar is now headed by professor V.Ye. Pogorelov. Over 2005—2009 years, Galyna Puchkovska was a Honorary Chairman of the School-seminar. Upon the motion of professor V.Ye. Pogorelov, since 2005, a satellite conference of the School-seminar is established — a summer mini-school of «Minor Academy of Sciences of Ukraine» with a hope to involve and encourage young generation to contribute to a development of science in Ukraine. The best Ukrainian schoolchildren winners of all-Ukraine competitions on physics are admitted to the summer mini-school. The kids not only attend lectures of noted scientists at the School-seminar, but present their own scientific research works.

Main topics of up-to-date scientific programme of the School-seminar include recent advances and developments in experimantal and theoretical methods of spectroscopy and its application to the studies of physico-chemical processes in solid state and soft matter objects, including nanoobjects and biological ones. Proceedings of the School-seminar were published in numerous books of collected papers, Journal of Functional Materials, as well as two special issues of SPIE Proceedings.

On September 29, 2010, professor Galyna Puchkovska passed away. To perpetuate the memory of Galyna Puchkovska and her contribution to world science, the Organizing Committee of International School-seminar "Spectroscopy of Molecules and Crystals" unilateraly decided to name the school-seminar after professor Galyna Puchkovska.

It is already 38 years since Galyna Puchkovska School-Seminar continuies to unite spectroscopists from different countries of Europe and the entire world, helps to establish new scientific contacts and develop new research projects, stimulates exchange of thoughts and ideas, and inspires new generations to work in science.

1
THEORY

PROPERTIES OF DIMERS AND TRIMERS
IN VAPOR AND IN LIQUID WATER

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Our work is devoted to investigation of clusterization in vapor and liquid water. The main attention is focused on the study of dimers, trimers and other linear associates, as well as hexagonal rings. For the description of interaction between water molecules the generalized polarization potential of Stilliger and David type is used. The parameters of they ground states are in details determined. The stability of these objects is investigated. The considerable attention is paid to their excitation states. For linear associates this question is equivalent to the consideration of vibration states of H-bonds. In particular, it was shown that only one transversal oscillation of H-bond is independent. Another its transversal oscillation is connected with longitudinal one, so we can speak about two hybrid oscillations of H-bond. It is established that all these results can be also obtained with the help of the multipole electrostatic potential including terms up to octupole moments.

The careful comparison with experimental spectroscopy data is carried out. The manifestation of clusterization effects in the temperature dependence of the heat capacity of liquid water is considered. It is shown that anomalously big value of the heat capacity is connected namely with transversal vibrations of H-bonds in water. The formation of dimers near the critical point of water is discussed. The internal rotation of water molecules around H-bond bonding them to dimer is discussed. In connection with this the strong manifestation of isotopic effect is predicted. The averaged intermolecular potential is built and its tight interconnection with thermodynamic properties of water are considered.

[1]. S.V. Lishchuk, N.P. Malomuzh, P.V.Makhlaichuk. Why thermodynamic properties of normal and heavy water are similar to those of argon-like liquids? // Phys. Lett. A. — 374 (2010) 2084—2088.

[2]. I.V. Zhyganiuk Generalized Stillinger-David potential // Ukr.J.Phys. — **56**, (2011) 225—232

FEMTOSECOND OPTICS OF THE ELEMENTARY WAVES PACKETS

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The main scope of this paper is to presend the method of the electromagnetic waves presentation without restriction of its duration. Besides it is advisedly to take into account specific features of electromagnetic signals. Then we use this representation for electromagnetic signal analysis and synthesis, solve some classical tasks for nonstationary electromagnetic wave propagation and diffraction. So it consists of such pasts:

1. Introduction.
2. Elementary waves packets (EWP) series.
3. Models and analysis of the optical signals.
4. Polarization properties of the EWP.
5. Nonstationary diffraction.
6. Interaction of the femtosecond optical pulse (FOP) with two level systems.
7. Conclusion.

SPECIFIC FEATURES OF METASTABLE STATES AT LIQUID-VAPOR PHASE TRANSITIONS AND NEAR THE BOUNDARY OF STABILITY

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The development of the ideas of modern phase-transition theory enables a consistent explanation to be given to the anomalous behaviour of various physical properties of liquids near the critical point. In recent years, this approach has been successfully used to study the specific features of the physical properties near the boundary of stability (spinodal) and near the lines of the first-order phase transitions.

The nature of spinodal and especially of metastable states has been actively investigated in recent years, in particular connecting with the theory of nucleation and spinodal decomposition. It is necessary to mention that the study of the metastable states in the immediate vicinity of spinodal is not an abstract theoretical problem. The specific features of metastable states at deep quenching to spinodal can be observed in a number of real experimental situations for such systems as Ising magnets, binary mixtures with a long-range intermolecular interaction, polymer mixtures with long molecular chains, binary alloys, and liquid crystals.

Therefore it is very important to discuss here such problems:

1. classification and stability criterion of metastable states;
2. equation of state in the metastable region;
3. calculation of critical exponents for a metastable fluid near the boundary of stability;
4. relaxation of the order parameter in the metastable region;
5. formation of new phases and its fractal structure.

DIFFUSION PHENOMENA IN LIQUIDS WITH REDUCED GEOMETRY

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The finite-size scaling theory was used to study the diffusion properties of individual liquids and binary liquid mixtures (namely, self-diffusion and diffusion coefficients, barodiffusion ratio, kinetic Onsager coefficients, isobaric compressibility, etc.).

Characteristics of barodiffusion processes in nanoscale liquid mixtures were examined with effects of the low crossover dimensionality and spatial dispersion taken into account. The dimensional crossover from 3D to 2D behaviour in biological objects like biomemranes was studied.

Comparison of theoretical results and experimental data for dependence of the water self-diffusion coefficient on the porous radius was examined with a qualitive and, under certain conditions, also a quantitive agreement between theory and experiment.

# ZONE OF REACTIONS AS A TOOL IN STUDYING THE SPACE-TIME STRUCTURE OF RELATIVISTIC NUCLEUS—NUCLEUS COLLISIONS

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In the collision of nuclei at high energies, a strongly excited system of interacting particles (fireball) is formed. A fireball is identified with the zone of reactions, i.e. with a space-time region, in which the reactions of particles occur. Hence, the zone of reactions must reflect the space-time characteristics of a fireball, and its study gives information about the evolution of the interacting system. While studying the evolution of a fireball it is important to know the size of regions, where the majority of various processes is running. Depending on a model describing the system, we can distinguish the regions of the formation of a fireball, its isotropization and thermalization, the creation of particles, the regions of a chemical freeze-out and a kinetic one, etc. This allows one to conditionally select the stages of evolution of the system and, hence, to obtain the limits of validity of phenomenological models used for the description of the complicated physical phenomenon, as well as to describe separate stages of development of the system in more details.

A zone of reactions is determined and then exploited as a tool in studying the space-time structure of an interacting system formed in a collision of relativistic nuclei. The time-dependence of the reaction rates integrated over spatial coordinates is considered. Evaluations are made with the help of the microscopic transport model UrQMD. The relation of the boundaries of different zones of reactions and the hypersurfaces of sharp chemical and kinetic freeze-outs is discussed [1]. Several time moments, which characterize specific stages in the evolution of the fireball, is proposed.
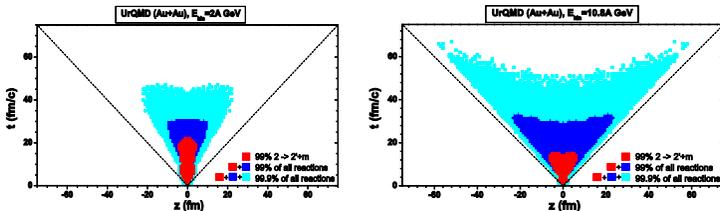
[1]. D. Anchishkin, A. Muskeyev, S. Yezhov, Phys. Rev. C **81**, 031902 (2010); arXiv:1004.0431 [nucl-th].

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EFFECT OF THE PARAMETRIC PROCESSES IN THE COMPETITION OF BACKWARD AND FORWARD STIMULATED RAMAN SCATTERING

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The question concerning the nature of stimulated Raman scattering (SRS) indicatrix asymmetry arose almost immediately after the SRS effect had been discovered. That was connected to the discovery of scattering intensity behaviour, namely the passing scattering intensity was usually greater than that of the opposing scattering. However, there is no universally recognized comprehensive explanation of the nature of the asymmetry nowadays.

New results concerning stimulated Raman light scattering indicatrix were obtained. Dependency of scattering asymmetry coefficient on the level of excess above the threshold of stimulated Raman light scattering was determined. The theoretical calculation proves that the existence of the stimulated Raman scattering indicatrix asymmetry is connected to presence of parametric processes.

The case is considered, when by z-axis, which coincides with the laser wave generation direction, Stocks and anti-Stocks components are generated. For anti-stocks component the conditions of phase synchronism are met. In the opposite direction only Stocks component is generated. A system of four coupled equations for laser wave electric field tension amplitude and fields of passing Stocks, opposing Stocks and anti-Stocks components correspondingly was solved. The obtained theoretical calculations were also corroborated by experimental results.

[1]. Stoicheff B. P. Characteristics of stimulated Raman radiation generated by coherent light // Phys. Lett.- 1963.- 7, №3.- P.186 - 188.

[2]. Shen I. R. The Principles of Nonlinear Optics, New York: Wiley, 1984. Translated under the title Printsipy nelineinoy optiki, Moscow: Mir, 1989.- 560 p.

EXCITATION PROFILES OF RESONANCE SCATTERING LINES FOR MOLECULES WITH DOUBLE MINIMUM VIBRATIONAL POTENTIALS

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Examples of calculation of the excitation profiles of the resonant Rayleigh and Raman lines corresponding to the transitions between states of the double-well potential of the vibrational subsystem of a molecule for some molecular model are given. Numerical solutions of the stationary Schrodinger equation for a particle in a double-well potential, both the ground and in the excited electronic state of a molecule are used. Obtained results demonstrate the possibility of using the formalism for the establishment of a mechanism of excited state intramolecular hydrogen bond proton transfer under the transformation of a molecule of monochromatic irradiation using the experimentally determined excitation profiles of the resonant light scattering data

PHOTOINDUCED NEAR-SURFACE MOLECULAR TRANSPORT GOVERNED BY FLUCTUATING COULOMB INTERACTION ENERGY

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The mechanism of directed substrate-parallel motion of molecules caused by photoinduced potential energy fluctuations is investigated. Unlike simplistic models (e.g., an on-off ratchet), the approach suggested implies that the necessary asymmetry of the potential energy can arise not only from the asymmetry of the substrate potential but also from an asymmetric distribution of the fluctuating charge density in the molecule [1,2]. The thus induced asymmetry of the potential energy governs the motion direction and enables, under certain conditions, its reversal at some frequencies of resonant laser pulses or temperature. These inferences are exemplified by the model charge distributions in the molecule and substrate, and the charge density fluctuations which are obtained by quantum chemical calculations for the realistic molecule of a substituted phenylpyrene compound on a model substrate (see Fig. 1).
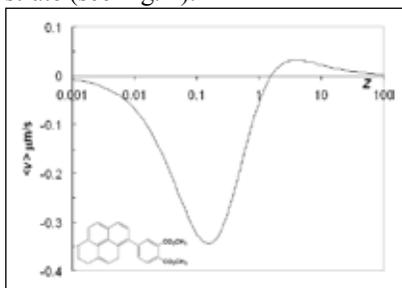
Fig. 1. The average velocity $\langle v \rangle$ of the photomotor based on the 1-[3,4-di(methoxycarbonyl)phenyl]pyrene molecule versus the parameter Z depending on the laser operating regime and temperature. The motion reversal occurs at Z about 1.6. The velocity is found with certain environmental characteristics and structural parameters of the substrate.

[1]. M. L. Dekhtyar, V. M. Rozenbaum. J. Chem. Phys. 134, 044136 (2011).
[2]. V. M. Rozenbaum, T. Ye. Korochkova, A. A. Chernova, M. L. Dekhtyar Phys. Rev. E (2011, to be published).

QUASIEQUILIBRIUM JUMPING DIRECTED MOTION IN A TIME-DEPENDENT POTENTIAL

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We consider the directed motion of a Brownian particle in a two-wells periodic potential with fluctuating barriers and wells governed by arbitrary functions of time, $v(t)$ and $u(t)$, alternating with the period τ [1]. In the framework of low-temperature kinetic approach, we arrive at the explicit formulas for the probabilities of finding the particle in the potential wells, average velocity of directed motion, input energy P_{in} and useful work P_{out} against additionally introduced stationary load force f. These formulas are essentially simplified for the quasiequilibrium regime of motion when $u(t)$ and f are small.

It is shown that depending on the mutual evenness or oddness of $v(t)$ and $u(t)$, the motion direction of a Brownian particle is reversed or not reversed under the reversibility of the direction of movement along the closed contour in the phase space of $v - u$ functions and the nondiagonal kinetic coefficients (proportionality coefficients between generalized fluxes and forces) are mutually antisymmetric or symmetric. In the adiabatic limit $\tau \to \infty$, average velocity is proportional to τ^{-1} in two cases: (i) the closed contour mentioned above has a nonzero area; (ii) functions $v(t)$ and $u(t)$ are proportional to each other (zero contour area) and contain intervals of fast changes with small durations τ_0 on the period τ of their variations. In these cases, the energy conversion efficiency $\eta = P_{out} / P_{in}$ tends to unit under the large barriers fluctuations $v(t)$. In the second case, the deviation of η from unit has two contributions, the first one decreases exponentially with increasing amplitude v_0 of function $v(t)$, and the second one is a small nonadiabatic correction proportional to $v_0^{-3/2}$. It is the nonadiabatic correction that limits the large efficiencies at large barriers fluctuations.

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THRESHOLDS OF LOCAL MODIFICATIONS OF A SOLID SURFACE AT LASER PROCESSING

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At modeling of process of interaction of radiation with substance the hydrodynamic model of a continuous medium was used. The problem has broken up on two. The first is a problem that describes the processes preceding to the destruction of the surface. The second is a problem that describes the processes of destruction of the surface. One of the main issues is a definition of threshold values of flux and the duration of pulse of electromagnetic radiation that separate an absence of destruction of the surface and the process when the surface destruction and a burning of corrosive torch are already possible.

During the solving of the first problem the relation determining the thresholds of destruction in dependence on the heat flux is received for the absorption coefficient of different materials. The ratios of threshold characteristics were analyzed for the different values of the absorption coefficient, namely for the unlimited (metals), almost zero (transparent semiconductors or dielectrics), finite (semi-transparent semiconductor and dielectrics) absorption and absorption that strongly depends on the intensity of radiation flux (so-called nonlinear materials). The threshold definitions comprise coefficient of overall dissipative losses, that allows to take into account the difference between volume properties of solid and its surface properties. This coefficient will allow to consider: the reflection coefficient, the surface absorption coefficient, which is usually different from the volume absorption coefficient, the surface scattering, which is related to the surface irregularity and depends on the ratio between the wavelength of incident radiation and the size of inhomogeneity of the surface, and also the changes of electron-phonon energy structure of the surface layer.

Second problem is related to a modification of a phase state the nano (micro) fields of a solid surface under irradiating. The principal factor restricting quality of the nanohandling is occurrence of a liquid phase and its incomplete removal in the course of this handling. Therefore we formulated one more threshold condition for a radiation flow. At realization of this requirement is realizable nanohandling (microhandling) of solid materials without formation of a liquid phase (melt).

During a solution of a problem of a problem of handling of a solid surface by a powerful pulse of laser radiation we have formulated the system of restrictions on intensity of a stream and duration of its action. The gained system of thresholds conditions gives an opportunity of prognostication of the necessary regimes for treatment by the laser pulse in concrete technological realization.

2
MOLECULES

# THE STRUCTURE OF EMISSION SPECTRA OF KRCL LASER (222 NM)

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Information about a structure of emission spectra for a laser is important for predicting abilities of the laser tuning. We have characterized a fine structure in the lasing spectrum of KrCl molecule in the area of 222 nm (45 030 cm^{-1}). Spectra were obtained by pumping mixtures $He/Kr/CCl_4(CF_2Cl_2)$ under the total pressure $0.3 \div 4.5$ atm in the electric discharge laser with automatic preionization. The emission spectra were photographed by spectrograph DFS-8 in the second order of 2400 line/mm diffraction grating on FUJI NEOPAN 400 film. The spectra were calibrated by emission of iron hollow cathode tube. Spectral data were processed in the way described in [1]. KrCl spectrum shows near 100 absorption lines. Some absorption lines were assigned to the absorption lines of $H^{35}Cl$ [2, 3]. The lasing was obtained on the molecule $^{84}KrCl$.

The assignment of emission lines for the iron hollow cathode tube for spectral areas 2460÷2505 Å, 4443÷4508 Å and 4920÷5010 Å were made. An atlas of emission lines spectra for the iron hollow cathode tube TSPK-type was created. Besides iron emission lines (Fe I, Fe II) we have seen emission lines of other elements (Ne I, Ne II, Ni I, Co I, Cr I, Cr II, Mn I). Mean square root error for characterized lines was 0.0004 Å.
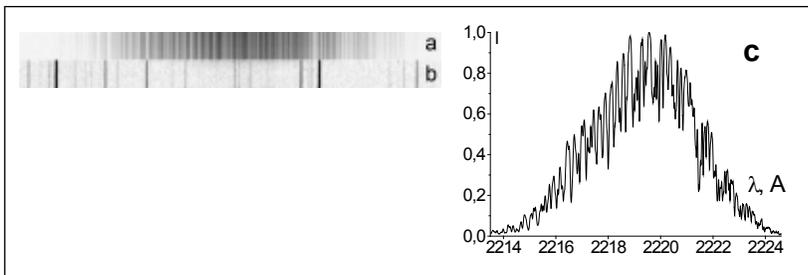
Lasing spectrum of KrCl (a), emission spectrum of TSPK tube (b) and microphotogram of KrCl lasing (c).

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A METHOD FOR STUDY OF EXCIPLEXES WITH PARTIAL ELECTRON TRANSFER

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A method for study of exciplexes with partial electron transfer between solute and solvent molecules is proposed. The method consists in comparison of the ratios of spectral shifts of different electronic transitions induced in molecules by the solvent under consideration and by the chemically inert solvents. The method is applicable to molecules that do not change their dipole moment on excitation. As an example, formation of exciplexes by molecules of benzene, phenanthrene, and naphthalene with water, ethers, and alcohols is studied. It is demonstrated that only high-energy states of the studied aromatic molecules participate in formation of complexes.

INTERACTION OF BENZENE MOLECULE WITH AQUEOUS SOLVENT AND WITH AQUEOUS SOLUTIONS OF ALKALI CHLORIDES

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Radii of cavities in solvents containing a benzene molecule are calculated using shifts of $S_1 \leftarrow S_0$ transition spectrum. A balance of pressing and exaggregation potential energies of a cavity in water containing benzene molecule is calculated in terms of quasi-spherical approximation. The exaggregation accomplishes by electrostatic reaction repulsive forces. Forces of microscopic surface tension and of dispersion interactions make the compression. It is shown that presence of ions destroying water structure leads to increase cavity size

NMR AND DFT STUDY OF HYDROGEN BONDING IN IMIDAZOLIUM-BASED IONIC LIQUIDS

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The ionic liquid 1-decyl-3-methyl-imidazolium bromide $[C_{10}mim]$ [Br], the neat material, and also dissolved (~0.01 mole fraction) in various dielectric media (acetonitrile, benzene, chloroform, dichloromethane, methanol, 2-butanol and H_2O) was studied using ^1H and ^{13}C NMR spectroscopy. The most important interaction in this compound is considered to be the $Br^-…H–C2^+$ hydrogen bond, which is formed between the anions and cations. The obtained results show that dielectric medium influence mostly the behavior of the $Br^-…H–C2^+$ bridge proton. The changes observed in ^1H and ^{13}C NMR spectra of $[C_{10}mim][Br]$ with increasing solvents polarity and temperature can be explained applying the model of the lengthening of the $H2…Br^-$ bond with the accompanying thickening of the solvation shell of bromine anion and C2–H bond contraction. The short-range order effects related to the configuration of neighboring dipoles of solvent molecules are more important for the solvation ability of small anions than the bulk solvent field effect. However, the solvents, molecules of which tend to associate via hydrogen bonding, can significantly affect the dynamics of anions.

SPECTROSCOPY OF ACRIDINIUM DERIVATIVES EXHIBITING CHEMILUMINOGENIC FEATURES

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Quaternary acridinium derivatives substituted in the central ring at the endocyclic N-atom and the opposing C-atom (in position 9) exhibit chemiluminogenic features, which are demonstrated in reactions with oxidants in alkaline environments [1,2]. In such conditions, acridinium cations are converted to electronically excited 9-acridinones which, upon radiative relaxation, emit light. Substances present in the medium can affect the intensity of emission. In such cases, chemiluminogenic acridinium derivatives can serve as indicators for the analytical determination of various entities [1,3]. Another possibility is to use acridinium cations as fragments of chemiluminescent labels, in which they are linked through a spacer to an active group capable of reacting with certain functional groups of macromolecules. Such chemiluminescent labels are commonly used in immunological diagnostics [1,3]. The utility of these indicators or labels depends primarily on the chemiluminescence quantum yield, which is governed by the structure of acridinium cation, particularly the type of substituent in position 9, the type of oxidant and the medium.

In the presentation, infrared, electronic and nuclear magnetic resonance data for numerous acridinium chemiluminogens that we synthesized in our laboratory will be shown and discussed from the point of view of the relations between the spectral characteristics and the structure and properties of the compounds. Furthermore, the relations between the probable mechanism of chemiluminescence generation and information emerging from spectroscopic investigations of acridinium cations will be considered. Finally, the structural – chemiluminogenic properties of these compounds will be analysed and the possibilities of designing analytically promising derivatives discussed [4].

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MOLECULAR AND LATTICE VIBRATIONS IN THE DESCRIPTION OF THE THERMAL BEHAVIOUR AND REACTIVITY OF GASEOUS AND CRYSTALLINE SOLID PHASES

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Each atom in a gaseous phase possesses three translational degrees of freedom. When atoms form a molecule in a crystalline solid phase, these degrees of freedom are transformed to $3n$ vibrational ones, where n is the number of atoms forming a molecule [1,2]. Of the $3n$ so-called normal vibrations, $3n-6$ (or $3n-5$ in the case of linear molecules) are molecular vibrations whereas 6 (or 5 in the case of linear molecules) are lattice vibrations. Apart from reflecting the unique spectral features of crystalline molecular systems, molecular and lattice vibrations determine the zero point energy of molecules and crystals respectively. As thermal processes take place predominantly as a result of excitation to higher vibrational levels, molecular and lattice vibrations reflect the thermal behaviour and reactivity of substances in gaseous and condensed phases [3].

The presentation will deal with the possibilities of identifying and determining the wave numbers of molecular and lattice vibrations, both experimentally and computationally. Examples will also be given of how experimentally determined or computationally predicted wave numbers are used to describe the thermal behaviour of crystalline solids, and also the kinetics of reactions occurring in gaseous and crystalline solid phases [2,3]. Correlations of the fatures predicted in the above manner with results of thermoanalytical investigations will be outlined. An attempt will be made to shed more light on the nature of thermal processes [4].

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NEW FLUORENE DERIVATIVE WITH EFFICIENT TWO-PHOTON ABSORPTION AND STIMULATED EMISSION DEPLETION FOR APPLICATION IN BIOIMAGING

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A comprehensive analysis of linear photophysical, two-photon absorption (2PA) and stimulated emission properties of new fluorene-based compound (E)-2-(3-(2-(7-(diphenylamino)-9,9-diethyl-9H-fluoren-2-yl)vinyl)-5-methyl-4-oxocyclo-   hexa-2,5-dienylidene) malononitrile (**1**) are presented. Linear spectral parameters, including excitation anisotropy and fluorescence lifetimes were obtained in a broad variety of organic solvents at room temperature. The degenerate 2PA spectrum of **1** was determined with a combination of the direct open aperture Z-scan and relative two-photon induced fluorescence methods using 1 kHz femtosecond excitation. The maximum value of 2PA cross section ~ 1700 GM was observed in the main long wavelength one-photon absorption band. One- and two-photon stimulated emission spectra of **1** were obtained over a broad spectral range with a femtosecond pump-probe technique and relatively high two-photon stimulated cross sections ~ 1200 GM were shown. A potential application of **1** in bioimaging was demonstrated via one- and two-photon fluorescence microscopy images acquired with incubated HCT 116 cells containing the dye encapsulated micelles.

IR SPECTROSCOPIC STUDY OF OZONE MOLECULE IN LIQUID ARGON SOLUTION

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Due to its ecological importance, ozone is a very well spectroscopically studied molecule in the gas phase. However, analysis of the vibration-rotational spectra of O_3, especially of the mixtures of isotopic-enriched ozones, is complicated because of strong perturbation of vibrational modes ν_1 and ν_3 by the Darling-Dennison and Coriolis interactions.

Advantages of dilute solution in liquid cryosolvent, such as liquid Ar, are relative narrowness of the spectral bands, weak perturbations of the intramolecular dynamics of solutes, and suppression of hot transitions from the thermally populated states. The experimental data on the band intensities and the transition dipole moments for such important molecule as ozone remains limited.

In this work, we studied IR spectra of $^{16}O_3$ as well as ^{18}O-enreached ozone molecules in liquid Ar solution at about 80 K. Frequencies and relative strengths for several vibrational transitions in ozones were measured and calculated. It was found that the strength of the ν_1 band of asymmetric C_s ozone isotopomers ($^{16}O^{16}O^{18}O$ and $^{16}O^{18}O^{18}O$) is significantly higher than for its symmetric C_{2v} modifications ($^{18}O^{16}O^{18}O$, $^{16}O^{18}O^{16}O$, $^{16}O^{16}O^{16}O$, $^{18}O^{18}O^{18}O$).

The data obtained are in good agreement with previously reported data [1, 2].

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FTIR STUDY OF INTRAMOLECULAR AND INTERMOLECULAR HYDROGEN BONDS IN SUBSTITUTED PHENOLS: "STRUCTURE-PROPERTY" RELATIONSHIPS

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Hydrogen bonds have a significant influence on the properties of organic molecules without changing their chemical structure. Hydrogen bonds can be classified into two types: intramolecular and intermolecular hydrogen bonds. Substituted phenols are the example of systems in which hydrogen bonds play an important role. Substituted phenols are the main fragments of many natural and synthetic antioxidants, food additives and drugs. These facts make actual task studying of the hydrogen bonds in these systems. FTIR-spectroscopy is one of the most informative methods for studying hydrogen bonds.

In this work, infrared spectroscopic study of hydrogen bonds in solutions of substituted phenols was carried out. Isomeric methoxy-, chloro-, nitrophenols, hydroxyacetophenones, di- and trihydroxybenzenes were investigated.

Stretching vibrations frequencies of intramolecularly H-bonded OH groups in the ortho-isomers of studied phenols were determined. Peculiarities of changes in the strength of intramolecular hydrogen bonds in substituted phenols due to molecules structure were studied. Obtained spectral parameters of intramolecular hydrogen bonds were compared with thermodynamic functions of their formation.

Stretching vibration frequencies of H-bonded O-H groups in complexes of substituted phenols with proton acceptors in an inert solvent were measured. The influence of the substituent structure and position on the spectral parameters of hydrogen bonding was analyzed. The regularities between structure of substituted phenols and their ability to intermolecular bonding were obtained. It was shown that the strength of the complexes of hydroxybenzenes with adjacent hydrogen bonds is significantly increased due to manifestation of the cooperative effect. In this work methods to account for the cooperativity of hydrogen bonds were proposed. Obtained data show that the cooperativity factors in complexes of catechol and propylgallate don't depend on the proton acceptor ability of bases. The spectroscopic data of hydrogen bonds in substituted phenols were compared with the antioxidant activity and pK_a of studied molecules.

REGULARITIES OF ORGANIC MOLECULES FLUORESCENCE IN SYNTHETIC OPAL PHOTONIC CRYSTALS

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Possibilities of controlling spontaneous emission by placing emitters into photonic band-gap structures (photonic crystals) and creating new effective light sources on the base of such structures are intensively studying [1]. The aim of this work is to expose regularities of laser dye and intramolecular proton-transfer substance fluorescence spectra in synthetic opals with various dielectric contrasts.

Synthetic opals constructed of SiO_2 globules with a mean diameter of about 260 nm were infiltrated with rhodamin G (R6G), pironin G (PG), astrofloksin (AF) and 2,5-bis(2-benzoxazolyl)hydroquinone (BBHQ) by soaking initial samples into proper substance solutions. The molecules concentration in solutions was no more than 10^{-3} M. Dielectric contrast in photonic crystals was changed by additional infiltration with a water-glycerin solution or immersive oil. Fluorescence of BBHQ was excited by radiation of nitrogen laser at 337 nm and LED Edixeon EDST-3LAx at 400 nm. Fluorescence of the other molecules was excited by radiation of LED Edixeon EDST-3LAx at 515 nm. Exciting radiation were directed at small angles to the (111) plane of samples in the "reflection" and "transmission" geometries. Fluorescence spectra were detected in the <111> direction by using modernized spectrometer DFS-12 in regime of photon counting with accumulation.

In accordance with the "golden Fermi's rule", modification of organic molecules fluorescence spectra in synthetic opals is determined by the density of optical states in the vicinity of photonic stop-band. Within stop-band region the inhibition of spontaneous emission was observed for all substances. If the wavelength, corresponding to the intensity maximum in spectrum of "free-state" substance, was shorter than wavelength, corresponding to the spectral position of stop-band center, the amplification of dye fluorescence at the high-energy edge of stop-band occurred. In contrary, a weak fluorescence was observed at the low-energy edge of stop-band without any amplifying.

Results obtained for BBHQ fluorescence spectra show the way to manage probabilities of irradiative transitions without and with proton transfer by choosing properly the stop-band spectral position.

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STRUCTURE AND NMR SPECTRA OF CYCLOPHANES WITH SMALL BRIDGES. WHY HYDROCARBONS WITH UNUSUAL SPATIAL STRUCTURE ARE WORTH STUDYING?

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Progress in organic synthesis in recent ca 50 years has allowed chemists to obtain hydrocarbons having spatial structures strongly departing from the standard ones that are in harmony with van't Hoff and LeBel hypothesis [1]. However, the question of applicability of such molecules (the problem of utmost importance, *e.g.* by writing grant proposals) is not always obvious. We were confronted with this problem when reporting a computational grant on cyclophanes like hexahydrosuperphane **1** [2] which should have a planar cyclohexane ring. Serendipity in which scientific discoveries find their ways to marketable applications will be shown together with stressing that, contrary to engineering, the aim of science is to get a better understanding of the world surrounding us and to satisfy our curiosity.
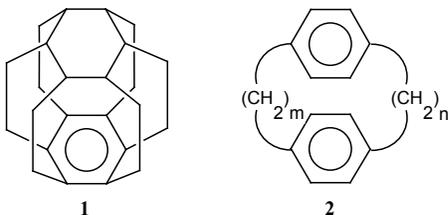
Cyclophanes with small bridges are interesting object in view of the non-planar structure of the aromatic rings and, when there is more than one of them, their location at close distances. The structure and NMR parameters of several cyclophanes were calculated and NMR spectra measured to analyse their interdependence. Some published [3,4] and novel results on the title molecules, in particular on their dynamic behaviour, will be discussed. At present (April 2011), the synthesis of hypothetical hexahydrosuperphane is carried out.

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# CHERENKOV SYNCHRONISM IN CONICAL EMISSION OF FEMTOSECOND BESSEL BEAMS

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The nature of conical emission (CE), a spectacular attribute of the femtosecond filaments and axicon-produced Bessel beams, is still a subject of discussion. The axicon-produced conical beams in weak nonlinear mode with clearly defined parameters have advantage over filaments to study the nature of CE.

Spectral-angular properties of CE excited by femtosecond laser pulses (150 fs, 802 nm, 300 µJ) axicon-focused   in 3 cm long water-filled cuvette have been studied. See the Figure for the photography of CE and angular dependence of the CE quanta energy.
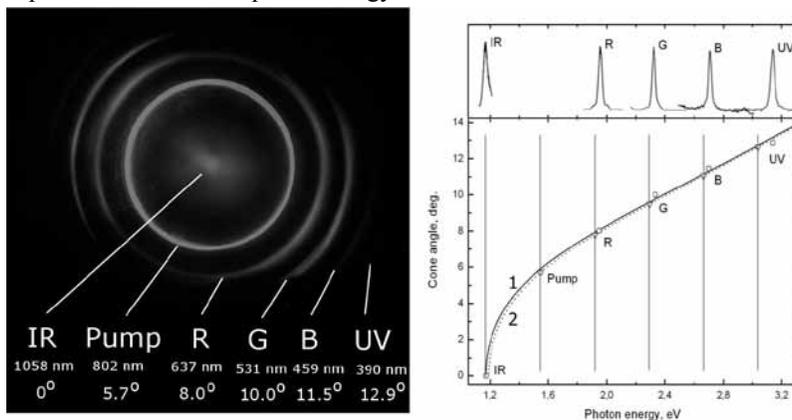
It is shown that angular dependence of the CE spectrum is governed by the Cherenkov-type synchronism. The discreteness of the CE rings is explained as due to the stimulation of signal IR emission along the beam axis in four-wave mixing process involving also two pump quanta and accompanied by R conical idler beam. Other conical beams G, B, and UV are caused by higher order multiwave mixing processes. Similarity of conditions of Cherenkov synchronism and that of Hawking radiation from the dielectric analogue of event horizon is also discussed.

THE IR STUDY OF COMPETITION BETWEEN INTRA AND INTERMOLECULAR HYDROGEN BONDS.

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The intramolecular hydrogen bonds are formed when one molecule contains both proton donor and proton acceptor groups in appropriate configuration.

The content of our contribution is devoted to comparison the properties of intramolecular and intermolecular hydrogen bonds and study the competition between both types of hydrogen bonds.

The difference in energy and IR spectra as well as thermodynamic stability of both types of hydrogen bonds will be discussed.

The competition between these types of hydrogen bonds appears natural when a molecule contains two proton donors as it is in secondary Mannich bases (**2**).
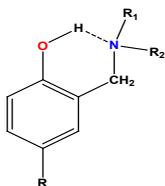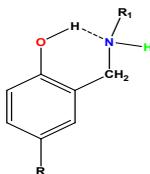
(1)   **(2)**

The spectra of such systems will be analyzed. Interesting effects of strengthening the intramoelcular intractions resulting from the formation of intermolecular hydrogen bond as well as specific stabilization of ionic forms in secondary Mannich bases will be presented, on the basis of spectra, quantum chemical calculations and crystal structures.

EVALUATION OF VIBRONIC INTERACTIONS IN CONJUGATE FLUORESCENCE AND FLUORESCENCE EXCITATION SPECTRA OF ALL-TRANS STILBENE AND DIPHENYLBUTADIENE IN RIGID MATRICES

V. Kompaneez, I.A. Vasilyeva

The fine-structure fluorescence and fluorescence excitation spectra of all-trans stilbene (SB) and diphenylbutadiene (DPB) are obtained at 4.2 K in an n-hexane matrix using the Shpolskii method. To determine the true relative intensities of the vibronic transitions of SB and DPB, we modeled conjugate fluorescence and fluorescence excitation spectra of SB and fluorescence spectra of DPB by a series of vibronic bands, each of which is the sum of a zero-phonon line and a phonon wing [1]. By choosing the necessary parameters, a nearly complete coincidence between the experimental and model spectra was achieved. In the case of SB, such a coincidence was obtained at a width of the zero-phonon line of 18 cm^{-1}, the width of the phonon wings of 144 cm^{-1} and at a Debye--Waller factor as great as 0.2. For DPB, the width of the zero-phonon line was 12 cm^{-1}, the width of the phonon wing of 108 cm^{-1}, and the Debye--Waller factor was the same. The large width and considerable intensity of the phonon wings indicate that the electron--phonon interaction between impurity molecules and the environment is strong. In addition, the calculated spectrum takes into account the deviations of the band maxima from their true positions upon intensity summation of closely spaced lines; consequently, the band positions are refined.

Based on the calculated spectra, the relative intensities of the vibronic transitions were determined. The parameters of the Franck--Condon (***a***) and Herzberg—Teller (α) interactions in the molecules considered are calculated [2]. For all the basic normal vibrations, the parameter ***a*** greatly exceeds α. Hence, the observed loss of mirror symmetry between the conjugate fluorescence and fluorescence excitation spectra of SB can be explained by the effect of high-energy states on the S_1 state.

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ALTERNATIVE HYDROGEN BONDING AND ESIPT PATHWAYS IN SUBSTITUTED NITROGEN-CONTAINING 3-HYDROXYCHROMONES

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Derivatives of the 3-hydroxychromone (3HC) family attract special attention. Exhibiting dual-band fluorescence owing to the proton transfer reaction in their excited state (ESIPT) [1], these molecules are highly sensitive to different parameters of their environment – polarity, H-bonding ability, viscosity etc [2]. This particularity has become the basis for development of a new approach in the applied fluorescent spectroscopy – ratiometric detection in physico-chemical, environmental and biological analysis.
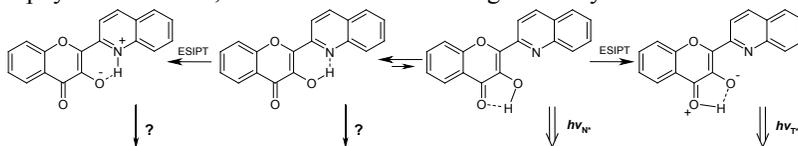
Traditionally, in the excited molecule of 3HC proton is transferred from the 3-OH group to the oxygen atom of the carbonyl group in position 4. However, certain derivatives of 3HC, possessing a heteroaromatic substituent in the position 2, introduce uncertainty in the above statement: the substituent's heteroatom could play a role of a second proton accepting center, which raises the question about the pathway along which the ESIPT process is realized in such a case [3-4].

In the present work we investigate the possibility of intramolecular H-bonds formation involving heterocyclic side moiety, as well as realization of an alternative ESIPT pathway along such bonds in several 3HC derivatives. General principles of multiband luminophores design with increased number of data reporting channels is discussed.

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PREDICTIONS BASED ON A COMPOUND-MODEL MORPHED POTENTIAL OF OC:HF

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A 6-dimensional vibrational-complete compound model morphed with radial shifting (CMM-RS) ground state potential generated for OC:HF is used to predict properties and test models of hydrogen bonding. The morphed adiabatic potential with both monomers in their ground vibrational states is characterized by an equilibrium rotational constant $B_e = 3345.68(30)$ MHz, equilibrium center of mass CO to center of mass HF distance, $R_e = 3.598(1)$ Å, and equilibrium dissociation energy $D_e = 1310(10)$ cm^{-1}. The generated CMM-RS potential can also be used to predict accurately numerous properties for OC-HF as demonstrated by: i) The prediction of the ground state dissociation energy $D_0 = 742.5(50)$ cm^{-1} and the 3-rd harmonic of the HF stretching vibration of the complex at 10893.90(50) cm^{-1}, both predicted within two standard deviations of error from the experimental data. ii) Generation of additional characteristics of this complex involving states that have not been previously investigated such as vibrational dependence of dissociation energies as well as structural and other properties. These include a comprehensive quantitative determination of first order inharmonic constants X_{ii} and X_{ij} and quantitative predictions of the corresponding band profiles. iii) Characteristics of the CMM-RS potential are also illustrated by comparison with prediction of properties made using previously published ab initio potentials. iv) Prediction of the characteristics of the CO-HF dimer. vi) The quantitative evaluation of models of non-covalent interactions. Specifically, in this case a comparison of the widely applied empirical Lippincott-Schroeder potential with the CMM-RS potential of OC-HF

FIELD-SUBSTANCE INTERACTION AND FORMATION MECHANISM OF CONTOURS OF MOLECULAR SPECTRA

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According to modern ideas, all the particles and the body are formed as a result of eddy processes and accumulation of physical vacuum. The energy density of physical vacuum is much higher than the energy density of the atomic nucleus. Therefore, structural and dynamical processes in condensed matter can not be discussed without taking into account the field-substance interaction. Taking into account these circumstances, a mechanism of formation of the contours of molecular spectra is proposed.

In molecular systems, as a result of the field-substance interaction on each individual molecule there induced rotational moments or spins (wave vector) of varying magnitude and direction, spatial distribution of which is random. The pattern of distribution can be described by statistical laws. The pattern of distribution of these quantities can be regarded as a phase portrait of the molecule's interaction with the environment or the wave function of response (WFR) of molecules. As a result of the interaction between the outer electrons of the molecules socialized electrons are formed. The interaction between them forms the oscillating WFR of electrons.

Oscillatory nature of WFR leads to oscillations of the center of gravity of the molecules, and the phase correlation between fluctuations in the center of gravity of the molecules forms the acoustic field of the environment, and the formation of an oscillating two-well adiabatic potential occurs. Acoustic wave propagation is accompanied by oscillation of the center of gravity of the molecules between two energy states. In the polarized spectrum of light scattering, they are manifested in the form of the shifted components relative to the frequency of the exciting radiation and the are called components of Mandelshtam-Brillouin scattering (MBS). The magnitude of frequency shift depends on the speed of propagation of acoustic waves in the medium.

The lack of central component in MBS indicates the absence of water molecules, which commits the translational Brownian motion. [O'Connor C.L., Shlupf J.P., J.Chem. Phys. 1967, v.47, p.31.92].
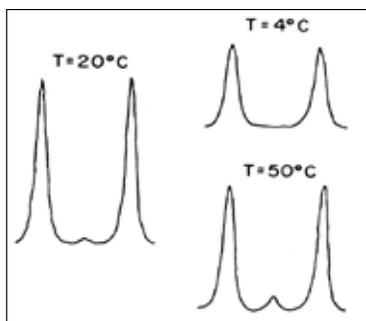
Fig.1. Spectrum of Mandelshtam-Brillouin light scattering (MBS) in pure water at three different temperatures.

Violation of the phase correlation of a single molecule with the environment leads to the formation of Brownian molecules, dynamics of the center of gravity of which is less affected by the adiabatic two-well potential. They form a central component of the MBS, and its intensity depends on the concentration of Brownian molecules in the medium. Increasing concentrations of Brownian molecules leads to the formation of the phase correlation between the fluctuations of their centers of gravity, which leads to the formation of the lower-frequency acoustic field. This process leads to a splitting of the central component of the MBS (in liquid helium), which means the appearance of second sound in the media.

Formation of Brownian molecules constitutes a violation of the symmetry of interaction of molecules with the environment. Therefore, as a result of the influence of the adiabatic two-well potential there is the reorientation of WFR of molecules from one equilibrium orientation state to another. In the spectrum of depolarized light scattering, this process manifests itself as a central Q-branch. Oscillating energy structure of WFR of molecules forms lateral O- and S-branches in the spectrum of Rayleigh light scattering (RLS). The superposition of these components forms the shape of the contour in the spectrum of the RLS. Shape of the contours in the infrared absorption spectra and spectra of Raman scattering (RS) should also be represented as a superposition of the central Q-branch and lateral P- and R- branches or O- and S- branches.

Energy structure of WFR of electrons in the ground energy level is manifested in the form of a broadband background spectrum of RS. The shape of the contour in the electronic absorption spectrum depends on the energy structure of the WFR of electrons. In the case of the formation of the phase coherence between the harmonics of WFR of electrons a coherent shell of WFR of electrons is formed. Energy structure of coherent shell of electrons is manifested in the form of a narrow and intense peak in the electronic spectrum, which is called the absorption edge. If at the transition of electrons from the excited electronic level to the main due to the coherent shell of WFR of electrons there is a delay of the re-emission of absorbed energy, this leads to the phenomenon of luminescence.

SPECTRAL (IR,NMR,UV-VIS) INVESTIGATIONS OF TRANSITION ELECTRON-RICH METAL HYDRIDES AND NONCLASSICAL COMPLEXES

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Spectral studies of transition metal hydrides in combination with quantum-chemical calculations allowed to know their interesting fundamental features. Transition metal hydrides possess two basic centers: transition metal atom and hydridic hydrogen bounded together and occurred to be unique proton acceptors. They can form two new types of hydrogen bonded complexes in interaction with proton donating molecules: with d –orbital of a metal atom (XH…M) and with partly negative charged hydride atom (XH…H) named dihydrogen bonded (DHB) complexes. We established reliable spectral (VTIR and NMR) criteria of them and the structure of proton transfer products via these hydrogen bonds. The products are classical cationic hydrides and non classical (η^2-H_2) ones, relatively. Our last investigations of the isostructure hydride series (M=Fe, Ru, Os) allow to find the peculiar features of electron rich metal hydride complexes. It occurred that metal site interaction with proton donor ($XH^{\delta+\cdots}$ M) can coexist with hydride ligand in DHB complexes leading to distortion of nearly linear geometry and can change proton transfer product from non-classical $M(\eta^2$-$H_2)$ for Fe and Ru to classical one for Os. The impact of each, M⋯H or H⋯H, depends certainly on ligand environment. It changes on descending the group in favor of the M⋯H interaction and we suggest this is a general trend.

RANDOM LASING AS MULTIMODE EMISSION OF A MULTIPLY SCATTERING MEDIUM

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Random lasing (RL) is the emission with laser-like behavior arising in a multiply scattering active medium under high optical pumping. This emission arises due to stay increasing of the emitted radiation in the sample because of multiple light scattering. Similar to conventional laser there is transition to emission with narrow spectrum. But this transition is not sharp and the radiation is unidirectional. Therefore the dominant conception of RL mechanism is amplified spontaneous emission (ASE), developed along random trajectories. However there are several attempts to represent RL radiation as the set of modes assimilated implicitly with random trajectories of scattered emitted radiation. But experimental confirmation of the modes existence was not obtained so far.

This work is aimed at experimental data obtaining to testify the mode existence and determine some their parameters. We investigated spectrum narrowing of radiation in concentrated suspension of BN and SiO_2 microparticles in rhodamine 6G (R6G) polyvynylacetate solution on pump intensity I_p. Dependencies of the spectrum width Dl and threshold pump intensity I_{th} on pumping beam diameter d, concentration of microparticles C_p and R6G molecules C_d were studied. The dependencies of the intensity I_m and wavelength l_m of RL spectral maxima and I_{th} on sample thickness h were investigated too.

The rate of the spectrum narrowing under I_p increase was shown to conform well with the value calculated from ASE conception only when one assumes sharp increasing of the radiation path in the sample under RL threshold. It is equivalent to the conception about circulation of RL radiation in confined space. It may be considered as experimental confirmation of RL modes existence. Without amplification these modes have low Q-factor and wide spectral contour. But Q-factor and running of mode radiation much increases when amplification a exceed loss k. It results in sharp narrowing of mode spectral contour. As losses differ for different modes the inequality a > k is satisfied progressively under I_p increasing and therefore the spectra of all the modes narrows rather smoothly.

Size of RL mode confinement reveals in dependencies $l_m(h)$, $I_{th}(d)$, Dl(h) and $I_{th}(h)$ as salient or extreme points connecting with diameter of mode confinement. This size decrease with C_p and particle refractive index and is order of 200mm (for SiO_2 suspension).

FILMING THE BIRTH OF A MOLECULE WITH X-RAYS

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A time-resolved x-ray diffraction study is presented to monitor the recombination of laser-dissociated iodine molecules dissolved in CCl4. The change in structure of iodine is followed over the terminal portion of the reaction path. Technical problems which appear at these short times are discussed in some detail. The solvent contribution is separated from the rest of the signal, and techniques of deconvolution are employed to reduce the effective duration of 100 ps x-ray pulses. They permit to monitor the recombination process up to the distances of the order of 2.7 Å. Images picturing the birth of I2 molecules are provided via temporally varying atom-atom pair distribution functions. The recombination process follows two reaction channels, located in the electronic states A/A' and X of the iodine molecule. Their time scales are of the order of 10 ps and 100 ps, respectively.

SPECTROSCOPIC STUDIES OF INTERMOLECULAR INTERACTION OF DIMETHYLPYRAZOLE AND DIPHENYLFORMAMIDINE WITH HYDROGEN HALIDES IN SOLUTION

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The spectroscopic characteristics and structure of hydrogen-bonded adducts formed by the bifunctional azo-compounds (AC) 3,5-dimethylpyrozole (DMP) or diphenylformamidine (DPFA) and strong proton-donor molecules of hydrogen halides HBr, HCl and HF were studied in solution by IR absorption spectra and quantum-chemical calculations. The obtained experimental spectra show that the proton transfer along the hydrogen bridge between HBr or HCl and basic nitrogen atom of the AC takes place with the formation of ionic pair $NH^+\ldots^-Hal$. The spectrum of the DPFA – HCl system in CH_2Cl_2 reveals strong band in the region 3200-2400 cm^{-1} with the centre of gravity near 2900 cm^{-1} [1]. The results of the B3LYP/6-31G** calculations for this system showed that the complex formed is characterized by the frequency of symmetric vNH^+ vibration of the cation involved in H-bond with the Cl^- anion, equal to 2850 cm^{-1}; this value is in good agreement with the experimental data. The interaction between DMP and HBr in CH_2Cl_2 demonstrates the similar spectral manifestations [2]. The addition of the excess of AC leads to the formation of the ionic 2:1 AC – HHal complexes; such complex includes $(AC)_2H^+$ cation with proton of N…H…N bridge located closer to one of the nitrogen atoms and two NH groups directed towards the Hal anion [3].

The experimental study did not give the convincing evidences of ionic structure for the DMP-HF system, and the quantum-chemical calculation showed that the hydrogen-bonded molecular complex with the hydrogen bridge N…HF is the most energetically and steric advantageous structure. Accounting for the effect of the solvent influence with use of the B3LYP/6-31G** level and the Tomasi model with dielectric permittivity $\varepsilon = 8.9$ (methylene chloride) yielded the following result: the potential minimum corresponding to the ionic form did not observed. This fact may be explained by very high dissociation energy of the H-F bond (D_{298} =135.3 kcal) in comparison with the values for H-Cl (103.1 kcal) and H-Br (87.6 kcal) bonds.

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OBSERVATION OF A METASTABLE CRYSTALLINE PHASE FORMATION IN 2-BROMOBENZOPHENONE

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In our previous works devoted to the vitrification process in the glass-forming benzophenone, 2-biphenylmethanol and salol we drew attention to their liquids being possible to cool below their freezing points without crystallizing; however their glassy phases crystallize on heating just after the glassy state becomes a liquid state (cold crystallization). Furthermore, it was shown that the cold crystallization tends to form the metastable polymorph [1-3]. The question arises is this observation a property of many supercooled systems, or is it a peculiarity of benzophenone, 2-biphenylmethanol and salol? In order to prove this, 2-bromobenzophenone (2BrBP) was chosen.

The crystallization behavior of supercooled 2BrBP as a function of time and temperature has been investigated by the infrared spectroscopy. We have monitored the C=O stretch vibrations, which are strongly influence by the changes in the structure. It has been found that the glassy 2BrBP crystallizes on heating into the metastable phase at 245 K. The splitting of the C=O mode in the metastable phase as compared to the stable phase has been observed. Also it has been found that there is a marked shift in the position of the C=O stretch vibrational band. The melting of the metastable phase has been observed at 303 K followed by the crystallization of the stable phase in 15 min. This is the first proof of the existence of polymorphism of 2BrBP. Also, the obtained results illustrate the well-known empirical rule (Ostwald's rule), which states that the phase that nucleates first is not necessarily the most thermodynamically stable phase, but is the one with closest free energy to the liquid phase [4].

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DIFFERENT POLYMORPHIC MODIFICATIONS OF PHENYL SALYCILATE

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An organic Phenyl salycilate or salol $((HO)C_6H_4CO_2C_6H_5))$ yielded polymorphic crystals: metastable (monoclinic) and stable (orthorhombic). There are many applications of salol, namely as a stabilizer for cellulosic and vinyl plastics, and also as an analgesic and antipyretic. In our previous study we have pointed out that glassy salol crystallizes to the metastable polymorph on heating (cold crystallization). The conditions of formation of different polymorphs have been clearly established in our previous investigations using Raman and IR spectroscopy [1, 2]. However, to our knowledge, a luminescence study of salol has not been performed so far. This observation motivated us to conduct the present study. The molecule of salol consists of two phenyl rings, which are connected by three single bonds through two, carbon and oxygen, atoms. The hydroxyl group is attached on one of the phenyl rings in the orto-position.

Fluorescence spectra measurements were performed by using a MPF-4 Hitachi spectrofluorimeter. The samples for the measurements were encapsulated in cylindrical glass tubes. The excitation wavelength was 363 and 340 nm. Luminescence spectra from both polymorphs of salol at low temperatures show a resolved progression involving the Raman and IR active $\nu(C_\phi\text{-OH})$ stretching mode. This means that the presence of an OH group in the 2-position on one ring asymmetrizes the molecule, localizing the electronic excitation to the OH-substituted ring. The $\nu(C_\phi\text{-OH})$ vibrational frequencies are on the order of 1250 cm^{-1} at 4.2 K. At room temperature both spectra show no sign of vibronic structure. The emission spectrum of the metastable phase of salol is red shifted by 750 cm^{-1} relative to the stable phase and is broader. The full width at half-maximum amplitude of the spectrum of the metastable phase is 1.4 times larger than that of the stable phase. The spectra of both modifications are sensitive to the changes in excitation wavelength 363 or 340 nm.

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STRUCTURE OF THE POLARIZED COMPONENTS OF 520 CM^{-1} BAND IN RAMAN SPECTRA OF QUINOLINE

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In some cases in Raman spectra (RS) peaks (maxima) of bands of the same vibrations do not coincide for different polarizations of the scattered light. Analogous situation we observed for 520 cm^{-1} band in quinoline. Parallel component at 20 ^{0}C is asymmetric in the high-frequency region. The shape of perpendicular component is of type that is usually corresponds to a band formed of two overlapping lines with approximately equal intensities. Due to a small magnitude of the depolarization ratio of the low-frequency band in parallel component a vibrational (isotropic) component is prevailed, and it determines the frequency of the peak of the resultant band. In perpendicular (anisotropic) component the overlapping lines are found to be rather equal by intensity. Usually, in such cases a non-coincidence of peak frequencies of parallel and perpendicular is observed. Quantum-chemical calculations showed that in the region of 520 cm^{-1} we really should have for a monomer molecule two closely spaced lines with wave-numbers 530 and 527 cm^{-1} (scaling factor 0,97) with depolarization ratio 0,61 and 0,26.

Previously we have suggested that the overlapping of closely spaced lines, which possess different depolarization belong to different molecular aggregations, can result in non-coincidence of the peak frequencies of bands. In this case the overlapping of bands occurs independently on aggregation of molecules, but the result appeared to be the same. In this case of the complicated 520 cm^{-1} band the difference in the peak frequencies is about 2 cm^{-1}. Dilution of quinoline by large amount of a neutral solvent leads to a narrowing of the overlapping lines, and thus they can be resolved separately.

RAMAN SPECTRA OF DEUTERO-METHANE (CD$_4$) IN MIXTURES WITH AR AND KR

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Spectra of spontaneous Raman scattering (SRS) of molecular gases contain extensive information on the vibrational-rotational energy states of molecules, as well as on intra- and inter-molecular interactions [1]. Obtaining of such information is of great importance both to deepen the fundamental understanding of the structure and dynamics of molecules and to use the obtained information for applied purposes.

Contours of the bands of isotropic Raman scattering (IRS) are currently the major source of information about the interactions and vibrational relaxation of molecules.

This paper presents the study of IRS spectra of the band ν_1 of deutero-methane in mixtures with Ar and Kr in the gas phase in a wide range of temperatures and pressures.

The aim of this paper was to study the factors influencing the formation of the band contours of the isotropic scattering of molecules of spherical tops in the Raman spectra of dense gases. Basic attention was paid to perform measurement and to identify the nature of the vibrational relaxation, due to the fact that by the present time this effect in the spectra of gases at moderate densities has been studied much lesser than the manifestation of the rotational relaxation.

IRS spectra were recorded on an apparatus constructed on the basis of the serial monochromator DFS-24. To carry out the temperature and the pressure studies we designed a special cell-thermostat, which is able to operate at pressures up to ~200 atm. and in the temperature range 77-370 K.

When the density is higher than Amaga the observed contour of the band ν_1 of CD$_4$ has a bell-like shape and is described by the Voigt function. In pure CD$_4$ at densities up to 20 Amaga at all temperatures the bandwidth within the error does not change [2]. With increasing density the band becomes more symmetric, and broadens. Along with the rotationally inelastic collisions, contribution to the broadening of individual rotational components, as well as swollen contour of Q-branch gives the

collisions, which change the character of the vibrational motion. It is comparatively easy to estimate the coefficient of broadening associated with the dephasing, if we know the dependence of parameters of the perturbing potential W on the vibrational coordinates of the active molecule. We calculated the broadening coefficients related to the dephasing of vibrations under the influence of dispersion forces. Changes in temperature leads to a qualitatively similar change in the coefficient of broadening for all the systems studied.

The calculation shows a weak dependence on the mass of the active molecule: when changing CH_4 on CD_4 the broadening coefficient should decrease by 9%. Experimentally it increases at about 3 times.

Experimentally observed non-monotonic temperature dependence of the broadening coefficient of v_1 band of deutero-methane is qualitatively described in the model [3]. Quantitative differences in estimates and experiment suggests that the mechanism does not exhaust the effect of broadening described in [3].

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AGGREGATION OF BENZENE MOLECULES WITH THE MOLECULES OF METHYL ALCOHOL AND FORMIC ACID

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Calculations and experimental studies of Raman scattering spectra show that there is a dimeric aggregation of benzene molecules with the molecule of methyl alcohol by use of π-electrons of the benzene ring. In this process H-active hydrogen atom of O-H group is oriented to the edge of the benzene ring (a distance along the normal to the plane of the benzene ring is 2.850 Å). The unusual position of H-active hydrogen atom is conditioned by interaction of two hydrogen atoms of the alcohol's methyl group with π-electrons of the benzene ring. In Raman scattering spectra the aggregation of molecules in the liquid state of the substance leads to broadening of the band of full-symmetric vibration with the maximum of 992 cm^{-1}, as well as to the shift of this band towards lower frequencies on ~1 cm^{-1}. The band of 992 cm^{-1} is narrowed more than twice at strong dilution of the benzene – methyl alcohol mixture by large amount of heptane.

The aggregation of benzene molecules takes place also with the molecules of formic acid by use of π-electrons of the benzene ring. As in case of the benzene – methyl alcohol mixture, H-active hydrogen atom of O-H group of the acid is shifted towards the edge of the benzene ring. The energy of benzene – formic acid dimerization is 9.24 kJ/mole.

INTERMOLECULAR VIBRATIONS IN LIQUID WATER AND THEIR MANIFESTATION IN IR ABSORPTION SPECTRA

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In our paper [1] it was shown that in spectra of Raman scattering (RS) something similar to the symmetric and antisymmetric vibrations of gas molecules is also preserved in liquid. As a result of intermolecular hydrogen bond, these vibrations are converted into broad bands, each of which, according to quantum-chemical calculations, are composed of a number of bands (with non-coincident frequencies of maxima) corresponding to different aggregates with the "symmetrical" and "antisymmetric" vibrations. Overlapping of these bands results as an experimentally observable wide band (~ 400 cm^{-1}) in water located in the region 3000-3800 cm^{-1}. The presence of different composition and different spatial structure of aggregates leads, as the quantum-chemical calculations showed, to a large number of intermolecular vibrations, the intensity of the bands of which is most significant in IR absorption spectra (in the Raman spectra these bands are weak). 400-1000 cm^{-1} band in IR spectra must correspond to these intermolecular vibrations. This frequency range is compared with the data of quantum-chemical calculations of the frequencies of intermolecular vibrations. We took the most intensive lines of intermolecular vibrations, which are non-coincident for aggregates of different composition and spatial structure (solid lines). As one can see, the calculated data are well reshapes the entire 400-1000 cm^{-1} band, and even describe the structure of the experimental band (lower-frequency region). In the process of comparison one should take into account the percentage of aggregates of different composition, but we, unfortunately, do not have this information.

Thus, intense intermolecular hydrogen bond and the difference in the properties of hese bonds in clusters formed in liquid water leads to appearance of wide $\Delta v = 340$ cm^{-1} and strongly shifted band shift with significant half-width.

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EFFECTS OF POLYMER MATRIX ON PHOTOSTABILITY OF ORGANIC DYES

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In the case of the lasers operated in the pulsed regime, the crucial parameter for their different applications is their service life period, which depends considerably on the dye stability in a solid medium during both its storage and running. Different factors affect stability of a dye in the polymer matrix. The probability of the interactions between dye molecules and active centers, leading to the destruction of the former in the polymer environment, is dependent on the mobility in this matrix.

The polymer matrices, characterized by an elastic state under normal operating conditions, are the most suitable for laser elements from different points of view. Such matrices required the minimum quantity of active centers for the stability of organic dyes.

This work presents the results of investigations on the effects of different elastic polymer matrices on photostability of organic dyes. The following three polymer matrices have been used. Polyvinylacetate was produced by means of radical polymerization; to obtain the corresponding samples, the dyes were incorporated into the finished polymer. Polyurethaneacrylate was doped by the dyes during its production process. And polyurethane was obtained by polycondensation method; the dyes were added also on its preparation stage.

The laser elements were based on the widely used classes of dyes, such as, xanthenes (Rhodamine 6G), pyrromethines (PM-597), polymethines (Astrafloxine), and phenalenones (F160). The polymer elements in a form of triplex, i.e. a polymer layer, placed between two glass plates, were made by different methods.

The effects of the polymer matrix type and its production technology on photostability of the samples have been studied. For the irradiation into the $S_1 \rightarrow S_2$ ground electron transition, the continuous emission of the neodymium laser second harmonic (532 nm) was applied. Ultraviolet light from an arc xenon lamp was used to investigate photostability in $S_1 \rightarrow S_n$ transitions. The dependence of the operation lifetime characteristics of dye laser elements on the polymer matrix type has been investigated in detail.

The affecting mechanism of the polymer matrix type and its production technology on photostability of the organic dyes in the polymer matrix has been discussed.

FTIR STUDY OF H-BOND CLUSTERING OF PROPANOL IN ARGON MATRIX: PRINCIPAL COMPONENT ANALYSIS AND CONCEPT OF RESONANCE BROADENING

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The FTIR spectra of propanol in argon matrix have been measured while heating the sample from $T = 11$ K to 30 K stepping by 1 K. Principal component analysis (PCA) and curve fitting have been carried out, the main attention concentrating to the region of propanol O–H stretching vibrations at 3000 - 3700 cm^{-1}. The peaks of monomers, two conformers of open dimer and the cyclic structures from dimer to pentamer have been resolved and studied in more details. The integral intensities of two peaks at 3564 and 3553 cm^{-1}, assigned to two conformers of the open dimers, have been processed in Arrhenius plot. The obtained slope 0.26 kJ/mol is comparable with the energy differences between the global minimum conformation of propanol and some other energetically higher structures evaluated by high level quantum chemical calculations. Analyzing dependences of the integral band intensities of various aggregates on temperature it has been deduced that monomers and dimers are in the initial clustering stage the main 'building bricks', which diffusion sustains the formation of the higher H-bond structures in the matrix. The full width at half height (FWHH) values for each band have been processed as the function of the aggregation number (n) and found that the FHWW is perfectly linear function of n for all cyclic aggregates $n \geq 2$. The resonance broadening has been proposed to be the most reliable mechanism of diffuse O–H stretching bands formation in the matrix isolated clusters.

FIRST EXPERIMENTAL STUDY OF COOPERATIVITY EFFECT IN COMPLEXES WITH INTRAMOLECULAR HYDROGEN BONDS IN GAS PHASE

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Cooperativity is one of the basic properties of non-covalent interactions. Particularly strong cooperative effects are manifested in the formation of hydrogen bonds. The cooperativity phenomenon means strengthening (weakening) of hydrogen bonding in a multi-particle complexes compared to the hydrogen bond between the same fragments, but in a binary complex. Cooperative effects significantly influence on the properties of polyfunctional molecules, which along with the intermolecular interactions formed intramolecular hydrogen bonds. Quantifying the cooperative effect in condensed phase faces the problem of taking into account the solvent influence. That's why determination of hydrogen bond cooperativity in the gas phase presents special interest.

In this work infrared spectroscopy investigation of phenol and 1,2-dihydroxybenzene with nitriles and ethers in the gas phase was carried out. Experimental data on the frequency shift of OH groups associated with proton acceptors show that the strength of hydrogen bonding in complexes of 1,2-dihydroxybenzene significantly greater than in complexes of phenol. This fact is due to the manifestation of the cooperative effect, which induced by the influence of intramolecular hydrogen bond of catechol on the intermolecular binding. In this work experimental method for the estimating the cooperativity factors in systems with intramolecular hydrogen bonds in the gas phase was proposed. The obtained values of the cooperativity factors in complexes of 1,2-dihydroxybenzene with nitriles and ethers are practically equal. Consequently, proton acceptor ability of the bases doesn't influence on the values of cooperativity factors. Results of experimental studies were confirmed by the quantum-chemical calculations using the DFT methods. It was shown, that theoretically obtained cooperativity factors of hydrogen bonds in complexes of 1,2-dihydroxybenzene with nitriles and ethers are in excellent agreement with experimental values. Cooperative effects lead to the strengthening of the intermolecular hydrogen bonds in complexes of catechol with nitriles and ethers by about 30 %.

THE SYNTHESIS AND X-RAY STRUCTURE OF THE 3-TRICHLOROMETHYL-4H-1,2,4-BENZOTHIADIAZINE-1,1-DIOXIDES AND 3-TRICHLOROMETHYL-4,5-DIHYDRO-1,2,4-BENZOTHIADIAZEPINE-1,1-DIOXIDES

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The compounds with 1,2,4-benzothiadiazine cycle are known to possesses of a wide spectrum of biological activity, e.g. the antiviral, antibacterial and hypotensive action. At the time seven-membered 1,2,4-benzothiadiazepine shows itself as an efficient diuretics and anticonvulsants. Plenty of related seven-membered heterocyclic substances of the benzodiazepine species are extensively used in medicine as anxiolytic and sedative agents.

A crucially new approach to the synthesis of the hard-to-reach 1,2,4-benzothiadiazines and 1,2,4-benzothiadiazines has been elaborated.

These substances were prepared under Fridel-Krafts conditions by cyclization of amidines formed by reaction of the N-chlorosulfonyltrichloroethanimidoylchloride with anilines or benzylamines.

The structure of the heterocyclic compounds obtained was confirmed by NMR ^{1}H, ^{13}C, IR, Raman spectral data and X-ray analysis.

It was shown that the conformation of the seven-membered cycle depends on nature of the substituent at the 4-th nitrogen atom. As a result of single-crystal X-ray diffraction it was found that in the most cases the molecules are characterized by the strong intermolecular hydrogen bonds which significantly influence on their spatial structure. X-ray diffraction has also shown that in crystals the chlorine-contained functional groups usually form intermolecular chains or nets by different types of short contacts which often include solvent or water molecules.

SPECTRAL MANIFESTATIONS OF INTRANOLECULAR SPIN-SPIN INTERACTIONS IN HETEROSPIN SYSTEMS

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Among the fundamental tasks related to a problem of structure and a dynamics of molecules, the central place occupy such intramolecular rearrangements where unpaired electrons of ligands are delocalized into metal ions changing the valency of the latter. Such rearrangements are commonly referred as valence tautomerism. As applied to compounds of first transition group, the above intramolecular processes lead to population $3d -$ orbital of metal with unpaired electrons. The investigations performed have shown that magnetic properties of compounds may alter dramatically owing to valence tautomerism [1, 2].

The present work reports the analysis of the ^{1}H NMR spectra in wide temperature range of semi-quinolate complexes capable of exhibiting the valence tautomerism effect. The study of proton paramagnetic shifts as well as the character of their temperature dependence has allowed the peculiarities of superfine interaction between resonating nuclei of ligands and unpaired electron localized on them to be established. The data obtained can be explained by NMR theory applied for paramagnetic systems [3]. The scheme involving compounds responsible for intramolecular exchange processes in the investigated semi-quinolate complexes has been proposed. It has been found that the intramolecular exchange assumes the obligatory presence of paramagnetic structure containing non-compensated electron spin localized on carbon atom of aromatic ring of the ligand molecule. The presence of such a structure leads to the appearance of satellite-like signals in the NMR spectrum. Apparently, this is the first experimental example of such manifestation of superfine interaction in the intramolecular exchange spin-spin interactions.

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RAMAN STUDY OF SUBSTITUTED
TERT-BUTYL-CALIX[4]ARENES

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Calixarenes are macrocyclic molecules that have cavity formed by phenol rings linked through methylene groups. Due to their unique architecture the compounds have ability to associate certain atoms or molecules forming supramolecular complexes. Therefore calixarenes are irreplaceable components for high-selective molecular and ionic receptors, separators, catalysts and so on. Selectivity to specific compounds can be changed by functionalization of calixarenes with certain substituents.

We have measured Raman spectra in solid state of a few calix[4] arenes functionalized with tert-butyl groups on the upper rim and different substituents (hydroxy, propyloxy, butyloxy) on the lower rim. The research reveals correlation between type of substituents and vibrational frequencies.

This work enables rapid analysis of calix[4]arenes for determination of type of substituents and purity of synthesized compounds.

DEGRADATION OF CHLOROPHYLL PHOTOLUMINESCENCE IN PLANTS

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Investigation of the chlorophyll photoluminescence (PL) spectra has been used for a long time in the ecological monitoring as one of the simplest contactless methods to obtain information about the plant functional state. In this work, it is shown that the PL intensity decreases with time rather rapidly, which can affect the obtained results.

The luminescence degradation effect is studied on the leaf fragments of the higher water plant *Vallisneria spiralis* L. at room and liquid nitrogen temperatures. The luminescence is excited by LGN-402 argon-ion laser radiation of 488 nm wavelength, the excitation density in the beam is about 200 mW/cm^2. The degradation curves are recorded at band peaks of the chlorophyll *a* PL spectra, whose positions at room temperature are 740 and 685 nm for the photosystem (PS) I and PS II [1], respectively.

The decreasing of the PL efficiency occurs rapidly enough, the intensity drops approximately by a half as early as from 1 to 2 minutes after the start of the illumination. At 685 nm (PS II), the degradation process runs slightly faster than that for the 740 nm band (PS I). The degradation of both the luminescence bands becomes slower at liquid nitrogen temperature.

It is shown that the intensity decrease dynamics is rather well described by a sum of two hyperbolic functions

$$I(t) = \frac{A_1}{1 + t/\tau_1} + \frac{A_2}{1 + t/\tau_2},$$

where A_1, A_2, τ_1 and τ_2 are constant values.

A slow restoration of the luminescent system is observed at room temperature after discontinuation of irradiation. No intensity restoration is detected at low temperatures.

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MANIFESTATION OF THE RESONANCE DIPOLE – DIPOLE INTERACTION IN THE IR SPECTRA OF FREON MIXTURES

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The IR absorption spectra of the cryogenic solutions C_2F_6 in CF_4 (T = 89 K, L = 2.02 cm) and CF_4 in C_2F_6 (T = 173 K, L = 0.5 mm) are studied. The band frequencies of the vibrational transitions accompanied by an excitation of strongly IR active modes v_3 (CF_4) and v_{10} (C_2F_6) are determined. The frequencies of the combination bands are collected in Table 1 for C_2F_6 (v_2+v_{10}) and Table 2 for CF_4 (v_1+v_3) in accordance with the Lorentz–Lorenz equation for solvents ($F_L=(n^2-1)/(n^2+2)$).

The linear dependences inherent in the induction interaction [1] are observed to be y=48(5)x-2054(1) for the C_2F_6 system, and y=60(9)x-2186(2) for the CF_4 system. However, the points, which define C_2F_6 in liquid CF_4 and CF_4 in liquid C_2F_6 systems, drop out of the common regularity.

The observed effect owes to the presence of the resonance dipole – dipole interaction (RDDI) in the studied systems.

To calculate the band frequencies, the program for modeling of absorption band shapes in the low-temperature molecular liquid spectra with an account for the RDDI [2] was used. The band shifts Δ are found to be: $\Delta (v_2+v_{10})$ = -12(3) cm^{-1} for C_2F_6 in liquid CF_4 (Δ_{exp} = -12(2) cm^{-1}), and $\Delta (v_1+v_3)$ = 21(2) cm^{-1} for CF_4 in liquid C_2F_6 (Δ_{exp} = 17(1) cm^{-1}).

Table 1

	gas	Ar	CF_4	NF_3	Xe
F_L	0	0.144	0.157	0.175	0.240
V, см$^{-1}$	2053.9	2046.5	2035	2046.5	2042

Table 2

	gas	Ar	C_2F_6	NF_3	N_2	Xe
F_L	0	0.144	0.132	0.175	0.129	0.240
V, см$^{-1}$	2186.1	2175.4	2193.4	2176.8	2176.5	2171.9

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MOLECULAR ORDERING IN SOME CARBANION DISUBSTITUED PYRIDAZINIUM YLID TERNARY SOLUTIONS

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The active solvent molecules are in a continuous competition to occupy the nearest places around the dipolar spectrally active molecules in the ternary solutions achieved in a mixture of two solvents; one active and one inactive from the intermolecular interaction point of view. In this way, the ternary solutions are non-homogeneous from the point of view of polar solvent concentration.

Carbanion disubstitued Pyridazinium ylids were used as spectrally active molecules in this study. The first solvation shell symmetry is directly dependent on the chemical structure of the solute and solvent molecules. The composition of the first solvation shell surrounding a spectrally active molecule is changed by the collisions due to the thermal motion and only the average statistic weights of the solvent molecules can be estimated by spectral means.

Pyridazinium ylids are zwitterionic compounds with a visible electronic band attributed to an intramolecular charge transfer from the carbanion towards the heterocycle. Being very sensitive to the solvent nature, the ICT band is an indicator regarding the binary solvent composition around the spectrally active molecule. By using the wavenumbers in the maximum of the ICT band, one can establish the average statistic weight of the each type of solvent molecules in the first solvation shell of the phthalazinium ylid molecule.

In our experiments, the average statistic weight of the polar solvent molecules in the first solvation shell is higher than the molar concentration of these molecules in the rest of the solution.

By using a cell model of the ternary solutions, the difference of the pair interaction energies between the ylid molecules and the molecules of the two solvents was estimated for four carbanion disubstitued Pyridazinium ylids.

In ternary solutions achieved by solvents in which the universal interactions have the same strength, the difference between the pair energies approximates the energy of the specific interactions the Pyridazinium ylids and the protic solvent molecules.

On the bases of a cell model of the liquids, the differences between the pair energies composed by one solute molecule and one solvent molecules in their ground electronic states was estimated in this study for four carbanion disubstitued Pyridazinium ylids.

ABSORPTION AND FLUORESCENCE SPECTRA OF THE «HYPERFLAV» MEDICATION

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In this work we present absorption, fluorescence excitation and fluorescence spectra of the "Hyperflav" medication produced by SIC "Borshchahivskiy Chemical-Pharmaceutical Plant" (Kyiv). This compound is used as a photosensitizer in the photodynamic diagnostics of cancer [1, 2]. Hyperflav contains hypericin the extract of St.-John's wort (Hypericum perforatum L.). Accordingly to the manufacturer it's less than 2% of hypericin in the final drug [3]. Hypericin is well known for its ability to accumulate in the morphologically altered cells and used as an effective photosensitizer in photodynamic diagnostics [4, 5].

Absorption and fluorescence spectra of Hyperflav in the visible region are very similar to the analogous spectra of hypericin. So we suggest that the bands in absorption and fluorescence spectra of Hyperflav in the visible region are caused by the presence of hypericin. On this basis we can assume that Hyperflav can be used as photosensitizer for photodynamic diagnostics. It also can be used in photodynamic therapy, since accordingly to the literature if it is present in the cells it can damaged morphologically altered cells under irradiation by certain light wavelength [6].

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OPTICAL INVESTIGATION OF SILVER AND COPPER IMPURITIES IN ORGANIC SOLUTIONS

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The present paper report the spectral properties of organic solutions activated with Ag^+ or Cu^+ ions.

The absorption, photoluminescence and photoluminescence excitation spectra of organic ($C_3H_8O_3$, C_2H_5OH, CH_3OH) aqueous solutions with impurity ($10^{-5} - 10^{-1}$ mol/l) of Ag^+ or Cu^+ ions have been investigated in the temperature range of 77 – 290 K. The solutions involved do not luminesce at room temperature, but at 150 – 180 K they strongly emit under UV irradiation.

The organic solutions activated with Ag^+ or Cu^+ ions are characterized by groups of three bands in both the absorption (excitation) and emission spectra. The long-wave emission band is a structural one and it can be ascribed to the $nd^9(n+1)s \rightarrow nd^{10}$ transitions in a free Ag^+ (or Cu^+) ion. The structure of individual absorption bands was also detected.

A deforming effect of polar solvents on absorption spectra of involved systems with Ag^+ (or Cu^+) ions is studied.

Analyzing the spectral characteristics of the Ag^+ and Cu^+ ions in the organic solutions confirms the validity of the ionic model of absorption (emission) centers in the systems presented.

IR SPECTRUM OF THE 2,3-DI-O-NYTRO-METHYL-B-D-GLUCOPYRANOSIDE AND ITS INTERPRETATION ON BASIS STRUCTURAL-DYNAMIC MODEL CONSTRUCTION BY DENSITY FUNCTIONAL METHOD

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Structural-dynamic models of the 2,3-di-O-nytro-methyl-β-D-glucopyranoside molecule are constructed by density functional method in bases 6-31 G(d). Energies, structures, dipole moments, polarizabilities, frequencies of normal modes in harmonic approximation and IR intensities have been calculated. Interpretation of IR absorption spectrum is presented in range 600-3700 cm^{-1}. Advantages of model, which was constructed, compared with model, which bases on using valence-force field method and valency-optical theory, are discussed.

SPECTRAL PROPERTIES AND POSSIBILITY OF THE DOUBLE PROTON TRANSFER IN THE MOLECULE OF BIS-FLAVONOL

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Design of new fluorescent dyes exhibiting multi-band fluorescence is very important in the framework of dynamic development of a new approach in the applied fluorescent spectroscopy – ratiometric detection in physico-chemical, environmental and biological analysis. To this respect, multiple 3-hydroxychromone derivatives are of particular attention due to the intramolecular proton transfer (ESIPT) process occurring in the excited state of their molecules [1].

Simultaneous increase of the proton donor 3-hydroxyl group acidity and the proton accepting 4-carbonyl group basicity are considered to be the main driving force of the ESIPT process. The first effect, however, has been shown to determine ESIPT photophysics [2].
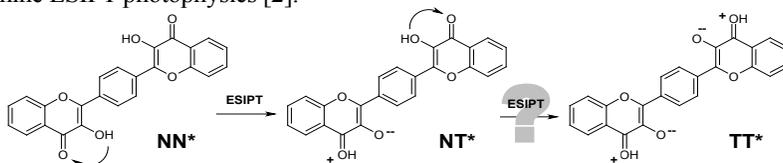
Beside the ratiometric response which is suitable for application in measurements related to natural and complex systems, multiband luminophores can be used for multiparametric probing due to the increased number of data collecting channels [3,4]. We hereby report spectral investigations of bis-flavonol, which is a structure with two five-membered H-bonded cycles potentially able to give rise to the double proton transfer in the excited state, and thus for the more complex fluorescence spectrum. The possibility of such a double transfer is as well discussed based on both *ab initio* theoretical modeling and spectral data analysis.

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LOW FREQUENCY RAMAN SPECTRA OF LIQUIDS ALKANS

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Low-frequency (LF) Raman spectra of liquid alkans from pentane (number of atoms of carbon n =5) up to heptadecane (n=17) in the region of 3 - 450 cm^{-1} are registered. These spectra processing is similar to that of LF spectra of water [1] in the region of 4-320 cm^{-1}. From Raman spectra of water the spectra of a dynamic susceptibility (DS) are calculate. It is well represented as the sum of four components: two lorentians, relaxation component and a luminescent background. The accuracy of the parameters definition is high [1]. In this report DS spectra are presented in the form of the only band placed in the region of frequencies from 3 up to 150 cm^{-1}. In the region of 3-8 cm^{-1} in most of the spectra (except for pentane) the edge of the peak of dynamic scattering is observed. For all the spectra the best accuracy of definition of parameters is in the region of 8 - 150 cm^{-1}, the spectrum being represented in the form of one gaussian without taking into account the central peak. The width of the line is much larger than the position of the frequency maximum. The dependence of the frequency of a maximum on the value of n is received. Clearly visible minimum of frequency is found out at n=7 (heptane). The correlation is clearly seen between the dependence on n of the width and that of the frequency. In particular, the maximum of the width at n=7 is clearly seen. The dependences of other parameters are received also. At decomposition on components in the region of 3-150 cm^{-1} taking into account the edge of the central peak, and the relaxation component being taken the same as for water, the shape of these curves for the frequencies and the widths of the basic line, is basically kept. However values of frequencies for most of the substances increase, and widths decrease. It is necessary to note, that in this case the dispersion of definition of all parameters increase very strongly. In particular, the dispersion of the intensity of the central peak is much larger than the average value. The width of the central peak for most of the substances is less than 1 cm^{-1}.

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SPECTROSCOPIC STUDY OF DYE SENSITIZERS DEGRADATION DURING SINGLET OXYGEN GENERATION

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In many applications, including photodynamic therapy efficiency of the dye sensitizer is assessed by the intensity of its visible photoluminescence because direct detection of singlet oxygen is rather difficult. We measured both the visible photoluminescence spectra of several dye sensitizers in the process of degradation and infrared photoluminescence of singlet oxygen. In Fig.1 photoluminescence spectra of metil-pheophorbide dissolved in chloroform ($CHCl_3$) at different stages of degradation are shown. Photoluminescence was excited with 75mW semiconductor laser operating at 405nm and registered by spectrometer equipped with InGaAs photodiode IGA-1300.

It was observed that reducing the intensity of photoluminescence of singlet oxygen at 1270 nm follows a decrease of the visible photoluminescence intensity.
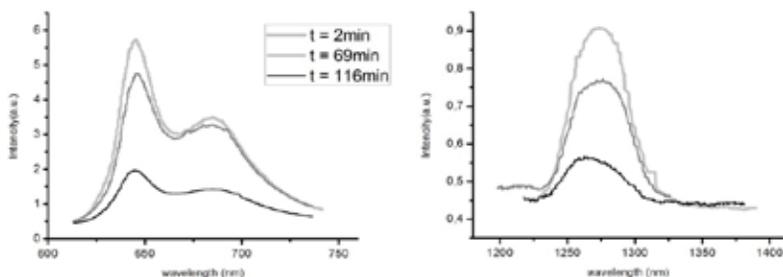
Figure 1. luminescence bands of the dye itself (640nm, 690nm) and singlet band (1270nm)

ON TEMPERATURE DEPENDENCE OF CONTOUR SHAPE OF COMBINATIONAL AND MOLECULAR SCATTERING OF LIGHT IN PARA-DICHLOROBENZENE

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The studies of the contour shape of combinational (CSL) and molecular (MSL) scattering of light are of interest since the contour shape is affected by inter-molecular interactions, different types of anharmonicity *etc*. This work is devoted to studying depolarized light scattering because this part of scattering is most of all connected with liquid and molecule structure.

To clarify a degree of community of the CSL and MSL mechanisms we investigated scattering in para-dichlorobenzene within the wide range of temperature 333–623 K (T_{melt}=325.3 K, T_{crit}=684.6 K).

An experimental setup was assembled on the basis of a high-aperture diffraction spectrometer DFS-12 with the lattice having 1200 *mark/mm*. A light source was argon laser LG-106 m with λ=488 *nm*. The CSL and MSL spectra were recorded in a mode of photon counting.

The studies have shown that the contour shape of the depolarized line of combinational scattering 1575 cm^{-1} in para-dichlorobenzene is described by one dispersion contour up to 30 cm^{-1} and the line shape of MSC by two dispersion contours up to 50 cm^{-1}. The half-width of the CSL line is significantly more (by 5 times for 333 K) than that of the MSC line. With the raise in temperature the half-width of the CSL contour increases; the intensity of the central part decreases. Unlike CSL in the MSL spectra a different picture is observed: temperature rising is accompanied by smooth contour widening up to 573 K only. Above this temperature a significant distortion of the contour shape takes place. This change in the shape mainly reduces to narrowing the MSL contour. Narrowing starts at the upper part of the central component (0–5 cm^{-1}) and further goes to (5–50 cm^{-1}). Within the whole range of temperature the intensity of the central part decreases. The integral intensity decreases as well.

For depolarized lines the essential temperature-dependent mechanisms of narrowing are hindered rotation [1] (up to 573 K) and oscillation anharmonicity. Line narrowing of the depolarized MSL part within the temperature range above 573 K in para-dichlorobenzene is associated with a contribution

of scattering by anisotropy fluctuations caused by vibrational motion of molecules. With the same the difference in the wide contour weight for high temperature from the theoretical value (α_2^{theor} =0.64, α_2^{exp} =0.77) should be connected. It can be assumed that the transition from more hindered rotation (up to 573 K) to more free one (above 573 K) should lead to changes in the wing shape of scattering line.

Such changes in a wing are predicted in [2]. Similar changes in the MSL contour we observed for a number of other liquids.

Comparison of the CSL and MSL data show that the central part of the CSL line decreases in intensity with liquid heating more than that of the MSL one; the peripheral part of CSL weakly depends on temperature while in the case of MSL the wing intensity (above 50 cm^{-1}) decreases with the raise in temperature.

Thus, it should be considered that the temperature behavior of contour width has the different nature for CSL and MSL. Widening for CSL is connected with decreasing resonance interaction of molecules, for MSL [1,2] with changes in a relative contribution of the vibrational mechanism and the hindered rotation one to scattering.

In our opinion, the available models cannot fully explain all the regularities. We think that it is necessary to take into consideration the changes in short range ordering and a degree (connected with the latter) of molecular field anisotropy to describe the temperature behavior of scattering.

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SOLVENT EFFECTS ON C=O STRETCHING VIBRATION FREQUENCIES OF AMIDES IN BASIC AND PROTIC SOLVENTS: ROLE OF COOPERATIVITY OF H-BONDS.

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Non-covalent interactions significantly influence on properties and conformational stability of biological systems. The main mechanism of this influence is the formation of intra and intermolecular hydrogen bonds (HB). Especially they are important in conformational stability of proteins and nucleic acids. The simplest models for investigation of non-covalent interactions in nucleic acids, proteins and peptides are amides. Today large quantity of models for analysis and estimation of influence of intermolecular interactions on IR frequencies are known.

In present study solvents effect on C=O stretching vibration frequencies of N-methylformamide (NMF), N-methylacetamide (NMA), N,N-dimethylformamide (DMFA) and its complexes with proton acceptors and proton donors were investigated. For analysis of solvent effects model [1] based on solvent parameter S_{VW} was applied. In the present work the method of determination of the cooperativity of H-bonds between amides and self-associated solvents, such as aliphatic alcohols and water were developed.

The first, absorbance of free molecules of NMA, NMF and DMFA in C=O stretching vibration frequencies were analyzed. It was shown that obtained C=O frequencies of these substances in inert and basic solvents linearly depend on solvent parameter S_{VW}, responsible for Van der Waals interactions. Measured frequencies of C=O group of amides in gas phase also lie on these dependencies. Sensitivity of studied carbonyl groups to solvent is decreased in the way NMF>NMA>DMFA. Deviations of frequencies from obtained linear dependencies were induced by HB formation and proton transfer. It was shown, that C=O stretching vibration frequencies in environment of strong proton acceptors (tertiary amines and etc.) fall out from linear dependence, due to formation of HB of NMF and NMA in complexes with proton acceptors (N-H...B). From calorimetric data new solvent parameter S_{DN} responsible for proton donor abilities of solvents was proposed.

Second, C=O frequencies of NMF, NMA and DMFA with complexes of aliphatic alcohols and water (C=O…H-O) were investigated. It was shown that obtained (C=O...H-O) frequencies of complexes (1:1) in proton acceptors and inert solvents linearly depend on solvent parameter S_{VW}. It was shown that frequency shift of carbonyl group in complexes of amides with monomers and clusters of water and alcohols are significantly differed due to manifestation of cooperative effects.

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HEAT TRANSFER IN SOLID CYCLIC HYDROCARBONS

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It is shown that in low temperature phase II the thermal conductivity measured under the atmospheric pressure changes as $\Lambda_p \mu T^{-1.15}$, while the isochoric thermal conductivity follows the dependence $\Lambda_V \mu T^{-0.8}$. In phase I the thermal conductivity measured under the atmospheric pressure decreases with a rising temperature as $\Lambda_p \mu T^{-0.31}$ and increases at isochores. This behaviour is quite typical for molecular crystals and is determined by several competing factors. The law $\Lambda \mu 1/T$ is obeyed when scattering involves only phonons and librons [1]. In low temperature orientationally-ordered phase II the isochoric thermal conductivity, which approaches its lower limit, follows a weaker dependence. The temperature dependence of the thermal conductivity measured under the atmospheric pressure is determined additionally by a sharp softening of the vibrational modes due to the thermal expansion of the sample. The latter also occurs in high- temperature orientationally-disordered phase I. The growth of the isochoric thermal conductivity at an increasing temperature in phase I may be due to the weakening phonon-rotation component of the heat scattering. In the orientationally-ordered phase of molecular crystals the total thermal resistance $W=1/\Lambda$ is a sum of the phonon-phonon and phonon-rotational components $W_{tot}=W_{ph-ph}+W_{ph-rot}$. The phonon-phonon component always increases with temperature. The phonon-rotation part is comparable in magnitude with W_{ph-ph} in ordered phases and tends to zero non a change to free rotation of molecules. W_{tot} reduces if W_{ph-rot} decreases more rapidly than W_{ph-ph} grows. It is shown that the experimental results can be described quanlitatively within the Debye model of thermal conductivity using the corresponding relaxation [1-2] and assuming that the phonon mean free path cannot be smaller than the half-wavelength.

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PHOTOPHYSICAL PROPERTIES OF ACRIDINE IN SOLUTIONS AND SIO2-FILMS. MATERIALS FOR OPTICAL SENSORS

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Optical chemical sensors that use luminescence, including changes of the radiation intensity, radiation wavelengths, spectral shape, and luminescence life-time possess high sensitivity and selectivity toward molecules of different analytes. The targeted search of compounds exhibiting sensor properties and the design of optical sensor materials on their basis is a topical task.

The acridine is suitable compound for creation of a material for an optical sensor. The spectral, luminescent properties, dipole moment in base and in excited states, photophysical processes of deactivation of excitation energy for acridine and for its protonated form were investigated experimentally and using quantum mechanical simulation.

It was shown that in this molecule the nitrogen of acridine cycle is a protonation site. The fluorescence maximum of protonated form considerably shifted in the red region and a fluorescence quantum yield increased up to 0,27 (for neutral form it is equal 0,03).

In results of carried out quantum-chemical calculations it was shown that for investigated molecule the lowest singlet and triplet states have pp* orbital nature and very weak fluorescence for acridine is result of strong singlet – triplet conversion. For acridine protonated form the rate constant of singlet – triplet conversion decreases on several degrees.

So considerable change of spectral-luminescent properties enables to use acridine protonated form as the active medium for detection of small amount of substances with the basic properties, for example ammonia. Suitable material for a matrix of an optical sensor is the material made from tetraethoxysilane (TEOS) received sol-gel method and doped with organic compound (acridine). Since in synthesis acid hydrolysis was used acridin was in protonated form in the final product. The sensor material was made in form of thin (< 1 mm) films by spin-coating method.

To study the capability of the received material to be a sensor for ammonia the investigation of spectral-luminescent properties of samples doped the acridine at contact with ammonia vapor was carried out. In result of interaction ammonia vapor with film surface the fluorescence intensity of protonated acridine fall down. It was caused by greater basicity of ammonia in comparison with a molecule acridine, that leads to transition of a proton from acridine nitrogen to a molecule of ammonia at their contact. The dependence of ammonia vapors concentration on fluorescence intensity was investigated.

INVERSION OF SOLITONIC-LIKE AND LOCAL ELECTRON TRANSITIONS IN STYRYL AND METHOXYSTYRYL DYES BEARING 2-AZAAZULENIUM MOIETY

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One of the most significant problems of the color theory of cationic polymethine dyes is the investigation of the dependency of the nature of the electronic transitions on the molecular topology. It is known [1,2] that the high intensive longwavelength absorption band is connected with $\pi \rightarrow \pi^*$ electron transition from the totally delocalized highest occupied molecular orbital to the molecular orbital of solitonic level (or level of the positive charge) with the large transition dipole momentum. In the dyes containing terminal groups with their own branched π-electron system the low intensive local transitions which involve the orbital, located only within the terminal groups, appear [3]. This could lead to the drastic transformation of absorption spectra, especially, in unsymmtrical dyes.
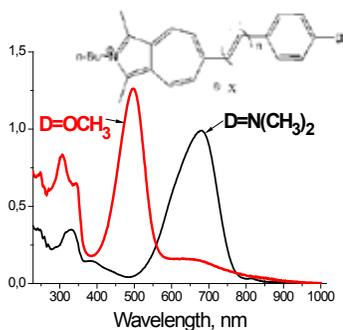
The report presents the results of both spectral and quantum-chemical investigation of the dimethylaminostyryl and methoxystyryl dyes bearing 2-azaazulenium moiety. It is shown that these extremely unsymmetrical cyanines differ between each other only slightly in the ground

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state with respect to the charge distribution and molecular geometry. In contrast, their spectral properties demonstrate the considerable difference between styryl and methoxystyryl – up to the inversion of the cyanine-like band and wide local band (Fig.1). The analysis of the quantum-chemical calculation gives that this spectral effect is connected with the different position of the local level in both dyes.

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STRUCTURE AND INFRARED SPECTRA OF ALIPHATIC AMINO ACIDS ISOLATED IN LOW TEMPERATURE INERT GAS MATRIXES

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We present results of the experimental observation of the nonionized natural aliphatic amino acids (glycine, alanine, proline, valine, nor-valine, leucine, isoleucine, β-alanine). The study has employed the low temperature matrix-isolation IR spectroscopy and the density functional theory (DFT) and *ab initio* calculations. 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. Energy of barriers separating the amino acid conformers was calculated at the MP2/aug-cc-pVDZ level. These data were used to determine for each amino acid the set of conformers which may present in the inert gas matrices. Assignment of the observed bands was performed based on calculated harmonic DFT/B3LYP/aug-cc-pVxZ (x=D, T) and anharmonic MP2/aug-cc-pVDZ frequencies.

We found that at least two conformers of each amino acid are present in the matrices: one with a bifurcated $NH_2 \cdots O=C$ H-bond (conformer **I**) and one with a $N \cdots H\text{-}O$ H-bond (conformer **II**). A trace amount of a third conformer with $NH_2 \cdots O\text{-}C$ H-bond (conformer **III**) was also detected. The conformational composition of the matrix-deposited nonionized amino acids was determined on the basis of observed and predicted IR intensities of the bands of different conformers. 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.

SPECTRAL PROPERTIES OF COUMARIN-CONTAINING EPOXYPOLYMERS: EXPERIMENTAL STUDY

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During the last decades PMMA has been widely used as a matrix for luminescent solar concentrators (LSC) mainly due to it resistance towards atmospheric conditions and good transparency in visible spectrum. Nowadays many works are devoted not to improvements of polymer plate's transparency, but to improvements of photo resistance dyes properties in matrix. Thus, the study in present work has been focused on development of new polymer composites for LSC that satisfy the high requirements.

As a polymer matrix we've used epoxypolymers that was synthesized using oligomeric diglycidyl ether of bisphenol-A and epoxy hardener such as trimethoxyboroxine (TMBOX). The choice of epoxypolymers as a matrix is caused by their high optical transparency in a wide spectral range and by possibility to change chemical structure and optical properties by suitable selection of initial monomers. Among a broad variety of dyes applied in LSC we've selected derivatives of coumarins that nowadays are well studied luminophors and thereby effectively used in various areas of engineering in particular due to the high stokes shift. The coumarin 504 (C504) was injected in epoxypolymer matrix in mixture with DCM [2-[2-[4-(dimethylamino)phenyl]ethenyl]-6-methyl-4H-pyran-4-ylidene]propanedinitrile.

Analysis of absorption and fluorescence spectra of studied dyes has revealed that DCM fluorescence spectrum occupy a long-wave region with respect to coumarin 504. The stokes shift of about 5517 and 1915 cm^{-1} is observed for DCM and C504, respectively. The certain positions of maxima in absorption and fluorescence spectra DCM and coumarin 504 allows to conclude that in such composition system the efficient energy transfer from donor (C504) to acceptor DCM is observed.

Also we've analyzed fluorescence spectra of certain dyes in epoxy polymer matrix at the range of concentration from 10^{-6} to 10^{-2} mol/l. It was established that the position of the bands in fluorescence spectra of

certain dyes does not change with concentration increase but the relative band intensities undergo significant. At the lowest concentration of DCM (1,2 μM) the DCM fluorescence spectrum practically coincides with the spectrum of pure dye C504 (λ_{max} = 480 nm). This implies that the incorporation of coumarin 504 in epoxypolymer matrix almost do not affect on fluorescent characteristic of dyes. The relative values of fluorescence quantum yield of studied epoxy polymers composites in the range of 520-780 nm have been measured.

   According to our experiments the increase of acceptor concentration accompanied by quantum yield increasing of epoxy polymer composite at stable concentration of it donor. However, this dependence is not in a good agreement for system with different donor concentration and constant acceptor concentration. Hence, in order to have high fluorescence quantum yield of polymer for each new dyes combination in epoxy polymer the new certain chromophore selection is required. In such a way, based on coumarin and DCM certain ratio selection the new combination of fluorescent dye is obtained. Thus the dye mixtures in epoxypolymer matrixes can be effectively applied such as fast-response fluorescence converters and in luminescence solar concentrators.

THE PECULIARITIES OF POLYMORPHIC TRANSFORMATIONS IN *N*-PARAFFINS (*N*=26, 28, 30, 32)

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It is known, that normal long-chain paraffins (*n*-paraffins) have a very different applications. They are used as components in the manufacture of tyres, rubber solutions, wood treatment products, adhesives, solvents for the seed oils extraction, rolling oil applications, household cleaners, detergents and in various aerosols formulations. That is why a precision study the physical properties of these compounds, namely their polymorphic transformations under different temperatures, is of a great importance.

In this work, the long-chain even-numbered *n*-paraffins with *n*=26-32 were studied by thermal X-ray diffraction (temperature step is tenths of a degree), infrared spectroscopy (temperature step is 1–5°), and differential scanning calorimetry (temperature step is 2°) in a sample heating melt cooling mode. The samples (Aldrich and Fluka product) are characterized by high homologous purity (99.0%). The molecular structure and the conformational composition of these *n*-paraffins in different states were found from their IR spectra. Differential scanning calorimetry (DSC) was used to determine the phase transition temperature.

We focused on the study of *n*-paraffins rotational dynamics. Under heating, n-paraffins undergo phase transitions from the crystalline state (*cryst*) to various rotational-crystalline states with different type of molecular thermal motion around their long axes. This diversity of crystalline modifications is dictated by the symmetry of the even- and odd-numbered chain molecules and hence by the packing of their terminal (methyl) groups in the crystalline structure. On the other hand, the contribution from an interplay between the intermolecular forces of the methylene chains (CH_2) in the layer and the interaction of methyl groups (CH_3) in the interlayer space should be taken into account. The stable and metastable phases, linear parameters their unit cells, as well as the temperatures of polymorphic transitions for *n*-paraffines are determined. The stages of thermal deformations and polymorphic transformations of long-chain even-numbered n-paraffins are discussed.

INFLUENCE OF DEFORMATION OF H_2O MOLECULE ON DEVELOPMENT OF H–O LINK DEVIATION

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The deviation phenomenon was revealed, because the problem was analyzed making use of the $3N$–matrix method (N is the number of atoms in a molecule), in which no preliminary assumptions about the character of the molecular force field are made.

The $3N$–matrix method is used where the frequencies of eigen normal vibrations are included into the evaluation procedure. It is found that the direction of the chemical bond O–H does not coincide with the direction of the straight line connecting the nuclei of the atoms O and H and that the deviation of the chemical bond is equal to 2° for a molecule H_2O in the gas phase.

For determination of force matrix of molecule H_2O we used experimental frequencies of normal vibrations of two isotopic modifications of molecule H_2O and D_2O.

As a result of computations the force matrix in this molecule is definite. That to define the characteristic of the force field in which the atom of hydrogen was found in this molecule a next method was applied. At the fixed position of atom of oxygen and one of atoms of hydrogen was calculated dependence of potential energies of molecule from direction of displacement of other to the atom of hydrogen in the plane of molecule on the fixed distance. This dependence in the polar coordinates has been named loop of deviation. Angle between these directions – the angle of deviation is amount 2°.

Preliminary deformation of the molecule was taken from the displacement from one equilibrium position one of atoms of hydrogen.

Research the loop of deviation of deformed H_2O molecule showed that the direction of maximum deviation loop is very sensitive parameter that responds to as the direction and amount of displacement of one of the of hydrogen atom, through which and by deformation of the molecule. Noticed that the deformation of the molecule due to displacement of hydrogen atom at a constant position of the oxygen atom followed by the change of equilibrium position of the other hydrogen atom.

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CRYSTALS

ELECTRONIC SPECTRA AND MAGNETISM OF FE-BASED SUPERCONDUCTORS

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The discovery of Fe based high T_C superconductors has initiated considerable interest to electronic structure, optical spectra and magnetic properties of these systems. Here we report results of theoretical and experimental studies of electronic and optical spectra, and magnetic properties of LaFeAsO and FeSe(Te) based systems.

Ab initio calculations of the electronic structure and optical spectra were performed by employing a full-potential LMTO method for a number of iron-based high Tc compounds. In order to shed light on the magnetic instability of the LaFeAsO and FeSe(Te) based systems, the DFT calculations of magnetic susceptibility were carried out in an external magnetic field. The band structure calculations revealed that the filling of conduction band near the hybridization "pseudo-gap" is predominantly responsible for magnetic and superconducting properties of LaFeAsO and FeSe(Te) systems. The calculated densities of electronic states and optical spectra are in agreement with available experimental data for the novel Fe-based superconducting systems.

Distinct peculiarities in the temperature dependences of the magnetic susceptibility $\chi(T)$ were observed in LaFeAsO(F) and FeSe(Te) systems. It is found, that these peculiarities are related to the antiferromagnetic transitions in the undoped LaFeAsO and FeTe compounds. For the $FeSe_{1-x}Te_x$ systems the initial effect of applied hydrostatic pressure is found to push up coordination unit elongation. We have revealed that magnetic properties and phases of FeSe(Te) are very sensitive to the height of chalcogen planes from the Fe plane. It is found that $FeSe_{1-x}Te_x$ systems are close to magnetic instability with dominating enhanced spin paramagnetism. The calculated values of the density of states at the Fermi level and paramagnetic susceptibility exhibit the strong dependence on the unit cell volume V and especially the height Z of chalcogen species from the Fe plane. The reasonable agreement between calculated and experimental values of χ at ambient pressure was obtained. The puzzling experimental pressure effect on χ was explained in terms of the pressure dependence of V and Z, the latter determining the dominant positive contribution.

SPECTROSCOPY OF FERROELASTIC LAYERED CRYSTALS ($CS_3BI_2I_9$): NEW PHENOMENA AND THEIR APPLICATIONS

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Ferroelastics is a peculiar new class of crystalline solids in which the spontaneous strain of a crystal lattice is appeared relatively of initial one as a consequence of structure phase transition from more symmetrical (paraelastic) phase into less symmetrical (ferroelastic) one. At cooling through the Curie point T_c (without any external action) the ferroelastic domains appear in the ferroelastic crystals in such a manner that the total strain of a sample (taking into account the stress sing in each domain) is zero. Such crystal partition into domains corresponds to the minimum of the strain energy of a crystal. One of ferroelastics is the $Cs_3Bi_2I_9$ layered semiconductor having high anisotropy of chemical bonding: a strong ion-covalent bonding in the separate layer sandwich and a weak Van der Waals interaction between the neighbouring sandwiches.

The review report deals with the experimental and theoretical studies of new phenomena registered.

The following problems were solved towards this purpose:

• The domain structure observations of $Cs_3Bi_2I_9$ were performed using the polarization microscope at heating and cooling regime.

• The separation of complicated contours of optical spectra with light polarization $E_\perp c$ into components was considered on the basis of Van Hove singularities.

• A nontraditional for the layered substances temperature shift of the fundamental absorption edge $Eg(T)$ of $Cs_3Bi_2I_9$ was found. It is shown that this shift is described very well by the Varshni formula.

• The transition region from 150 to 220 K was registered. It is shown that this region may be identified as the heterophase structure region where ferroelastic and paraelastic phases coexist.

• A change of exciton-phonon interaction from a weak to strong as temperature increases was found. The effect is explained on the basis of

a model which takes into account the reconstruction of the crystal lattice from non-layered to layered one.

• The temperature value T* =150 K may be considered as characteristic one below of which the crystal loses the nature of layered substance.

• Raman spectra of $Cs_3Bi_2I_9$ were studied in heating regime over temperature range 5-300 K but any soft mode or softening of modes were not observed. The interpretation of Raman spectra is given.

• The structure phase transition in $Cs_3Bi_2I_9$ at $T_c = 220$ K was registered. It is shown that this transition is the first order transition which is close to the second order one.

• A new giant thermodynamical optical effect near the ferroelastic phase transition point was found and explained on the base of Landau-Khalatnikov theory.

The optical active devices on the base of the phenomena found are proposed.

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COMPARATIVE PHOSPHORESCENCE SPECTRA OF SINGLE-BROMO-SUBSTITUTED BENZOPHENONE ISOMERS

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Substitution of a single hydrogen atom in the benzophenone molecule at three essentially different positions entails crucial changes in the molecular conformational parameters as well as in all macroscopic properties such as crystallization, crystal structure, luminescence, ability to form vitreous and polymorphic states, etc. Thus, the molecule of 4-bromobenzophenone (4Br-BP) in the free state is slightly asymmetric whereas the 2Br-BP and 3Br-BP molecules are strongly asymmetric, especially the former. Other relevant properties are listed in Table below.

Property	Unsubstituted		2Br-BP	3Br-BP	4Br-BP	
Shape of molecule in the free state	Symmetric		Strongly asymmetric	Substantially asymmetric	Slightly asymmetric	
Crystallization peculiarities	normal		Strong reluctance to crystallize from melt	Small crystallites irrespective of growth method	normal	
Propensity to vitrify	easily		easily	none	none	
Propensity to polymorphism	Two polymorphs		none	none	Two polymorphs	
Structure	Monocl C2/c	Orthorh. $P2_12_12_1$	Orthorh. $P2_12_12_1$	Monoclinic $P2_1/a$	Ortho Pbca	Tricl. P1
Excimer	none		yes	Very likely	none	
Exciton transport	Not known		normal	noexistant	Not known	

The crystal structure is strongly dependent of the respective molecular structure. Other physical properties, which can be experimentally studied by spectroscopy methods, depend as strongly also on the molecular shape in the electronically excited states.

In this comparative overview report, the reasons behind the cardinal differences in the physical properties and phenomena in the bromo-substituted benzophenones are analyzed within the "structure-properties" approach.

ELECTRON SPIN RESONANCE IN FERROBORATE $NDFE_3(BO_3)_4$

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The AFMR spectra of the $NdFe3(Bo3)_4$ crystal are measured in a wide range of frequencies and temperatures. It is found that by the type of its magnetic anisotropy the compound is an "easy-plane" antiferromagnet with a weak anisotropy in the basal plane. The effective magnetic parameters are determined: anisotropy fields H_{a1}=1.14 kOe and H_{a2}=60 kOe and magnetic excitation gaps d=101.9 GHz and d1=23.8 GHz. It is shown that commensurate-incommensurate phase transition causes a shift in resonance field and a considerable change in absorption line width.

LUMINESCENCE SPECTROSCOPY AND ELECTRONIC STRUCTURE OF $KZr_2(PO_4)_3$, $KBiZr(PO_4)_3$ AND ZrP_2O_7 CRYSTALS

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Phosphate crystals of alkali and four-valent cations are intensively studied as perspective luminescent materials for various scientific and technological applications [1, 2]. However at present, there is a considerable lack of scientific understanding of the nature of intrinsic emission and peculiarities of the excitation energy relaxation in these compounds. In this work we present results of experimental studies on VUV spectroscopy of undoped $KZr_2(PO_4)_3$, $KBiZr(PO_4)_3$ and ZrP_2O_7 crystals together with results of theoretical calculations of their electronic structure.

Polycrystalline samples of three crystals were synthesized by spontaneous crystallization method. Photoluminescence (PL) and PL excitation spectra were obtained at 4.2, 77 and 300 K. Luminescence was excited by radiation from the N_2-laser, diode pumped lasers and the powerful xenon lamp. The luminescence was registered using spectrometers, which cover wide spectral region. The VUV-excited luminescence and reflection spectra were studied on SUPERLUMI station at HASYLAB (DESY), Hamburg, Germany in 4 – 25 eV excitation energy region.

The electronic structure calculations of perfect $KZr_2(PO_4)_3$, $KBiZr(PO_4)_3$ and ZrP_2O_7 were performed by the Full potential Linear Augmented Plane Wave (FLAPW) method realized in Wien2k program package [3]. Partial densities of electronic states, components of the dielectric tensor, reflectivity and absorbance spectra are calculated and compared with appropriate experimental data. The origin of intrinsic emission bands and formation of the luminescence excitation spectra of investigated crystals are clarified using obtained experimental and theoretical results.

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LUMINESCENCE CHARACTERISTICS AND ELECTRONIC STRUCTURE OF THE SET BI-CONTAINING PHOSPHATES AND MOLYBDATES

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Oxide compounds, in particular molybdate and phosphate crystals are well-known as promising host for rare-earth ions. Origin of the intrinsic emission bands for these crystals had attracted much less attention than luminescence properties of the doped crystals.

Understanding the origin of emission bands in complex oxide compounds can be significantly improved by a combination of experimental spectroscopic studies in the different region of luminescence excitations and theoretical calculations of the electronic structure carried out for the set of genealogically connected hosts.

Undoped compounds $BiPO_4$, $K_3Bi_5(PO_4)_6$, $K_2Bi(PO_4)(MoO_4)$ and $K_5Bi(MoO_4)_4$ were synthesized by spontaneous crystallization method. The luminescence was studied on SUPERLUMI station at HASYLAB (DESY), Hamburg, Germany in $4-25$ eV excitation energy region and under visible laser excitations. Electronic structures are calculated by the FLAPW method realized in Wien2k program package. [1]

Emission spectra obtained under synchrotron radiation of each studied compound consist of complex bands in "yellow" spectral region (550-750nm). Strong temperature quenching obtained for these emission bands. All samples reveal comparatively weak luminescence band in "blue" region (400-500nm) under excitation with nitrogen laser (λ_{exc} =337.1nm) and T=300K. When temperature decreases to 77K, intensity of the "yellow" band dominate in spectra.

Calculation of the electronic band structure and optical properties were performed for all investigated compounds. Results of theoretical calculation were compared with experimental data. Origin of the emission bands discussed considering experimental spectra and theoretical calculations.

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INFLUENCE OF THE RE-DOPING ON MATRIX EMISSION OF THE LEAD TUNGSTATE CRYSTALS

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The lead tungstate $PbWO_4$ (PWO) crystals were intensively investigated during two last decades in connection with their application as scintillators for Large Hardron Collider. Doping of the lead tungstate crystals by the RE ions significantly improves transmission in the short wave length region and radiation hardness of the PWO. At the same time relations between the effects of the RE ions on the PWO characteristics are still under discussion. The investigated PWO crystals were grown by the Czochralski method. Impurities were added into the crystals using the RE_2O_3 oxides (Eu, Yb, Pr oxides). Their concentrations in the blend were 5×10^{-2} wt %.

Luminescence spectra of the un-doped PWO crystal obtained at 10 K consist of the band in 350 – 700 spectral region with maxima at about 460 and 470 nm at 300 and 270 nm excitations, respectively. For the Eu^{3+}-doped PWO crystals these maximums are 460 and 455 nm; for the Pr^{3+}-doped and Yb^{3+}-doped PWO crystals these maximums are 445 nm for the both noted excitations. Three bands with maximums at 520, 570 and 610 nm form the luminescence spectra at 320 nm excitation for the un-doped and RE-doped crystals. Differences in the maximum positions obtained for the main band can be explained by complex character of this band. It is well known, that emission spectra of the PWO crystals consist of the blue, green and orange-red emission. Obviously, the main band is complex and contains more than three spectral components. Their relative contributions depend on crystal quality and composition. This dependence causes shifts of maximum of the main band for the un-doped and RE-doped crystals. In order to find all spectral bands contributing in the total luminescence spectra we have carried out breakdown of the obtained spectra on Gauss components. The luminescence spectra measured at 10 K and various excitations can be presented by the several bands those are the same for of all the investigated crystals. It is clearly seen, that RE-ions influence on the redistribution of relative contributions of these bands in the total spectra. We assume that adding of the RE ions changes concentration of several defects in the crystal lattice and therefore leads to redistribution of content of emission centers responsible for each type of emission. Assignment of various types of defects to the obtained spectral components is discussed.

The samples were grown at the Physics Faculty, Lviv National Ivan Franko University, Lviv, Ukraine in the laboratory headed by Prof. M. Pashkovskyy. Experiments with synchrotron radiation were done at SUPERLUMI station at HASYLAB (DESY) in Hamburg, Project Nr. II-20080221.

SPECTROSCOPIC CRITERION FOR EXISTENCE THE NEGATIVE PERMITTIVITY

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Anomalous dispersion region of electromagnetic wave propagation, particularly, when the dielectric permittivity becomes negative is a subject of increased attention due to such fundamental issues as the anti-reflective surfaces development and metamaterials synthesis. Despite the long history of spectroscopic studies of negative permittivity it is leaves unresolved the question of negative dielectric properties quantification.

The influence of the polar vibrations damping on the negative permittivity values in anomalous dispersion region we have analyzed in our work. It is shown the existence of the critical dumping which is caused the full disappearance of negative dielectric permeability. It is the vibrations damping effects have a decisive impact on both the minimum DP value and the spectral range narrowing of the negative DP existence area relatively to T-L splitting of the phonon frequencies in polar crystals. Based on the model of crystal with one oscillation we obtain the simple quantitative criterion in form of inequality between the damping constant and phonon T-L frequency splitting as:

$$\Gamma < \left(\omega_L - \omega_T \right) \text{ or } \frac{\Gamma}{\omega_L - \omega_T} < 1 . \qquad (1)$$

Our analysis based on these inequalities makes it easy to predict the presence or absence of negative DP. Advantage of criterion (1) to predict the negative DC area existence is that it can be used for the analysis of highly complex phonon absorption spectra as is shown in our report.

Anisotropy effects on the negative dielectric permittivity (DP) formation in the frequency region near the phonon lattice vibrations are considered using three crystalline modifications of boron nitride. Quantitative data on frequency intervals and negative DP values are presented for all anisotropic modifications. It is shown that anomalous dispersion of the refractive index falls to $0 < n < 1$ in the presence of negative DP, but always leaves $n > 1$ in the absence of negative DP. The significant role of the polar vibrations damping to determination of the real limits of negative DP region is clarified, especially for crystals with symmetry lower than cubic.

EXTREMELY LOW IR REFLECTION BANDS IN CRYSTALS

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The anti-reflective covers and its creation possibility for the entire electromagnetic spectrum now mainly associated with the synthesis of metamaterials, which would have a negative refractive index, resulting from the presence of negative dielectric permittivity (DP) ε and magnetic permeability μ. As well known the negative DP can be found in the T-L splitting of polar phonons and this area can be investigated by standard methods of IR and Raman spectroscopy. Traditionally, the processing of reflection spectra of crystals in the far infrared (i.e. terahertz) range usually limited of parameters analysis of polar vibrations, which formed near the reflection picks and not paying adequate attention to reflection minima in addition these dips are often hidden in the instrumentation noises.

Dispersion analysis (DA) method as shown in our work is quite correctly describes the main features of reflection spectra with observed in the experiment and so he laid the basis for our calculations of the minimum reflection. We use the boron nitride for next modeling as this crystal has the simpler spectrum for analysis.

The physical features analysis to describe formation the regions with extremely low reflection of electromagnetic radiation in the terahertz and far infrared ranges are presented and these regions should be observed in many experimental studies. It is shown that in case of sufficiently small damping of polar phonon the spectral bands with almost complete reflection disappearance ($R < 0.01\%$) are formed and we name these bands as antireflection channels (ARC). ARC located outside the region of negative dielectric permittivity, and the minimum reflection is shifted above the frequency of longitudinal oscillations by the value depends on the basic parameters of the polar vibrations.

The appearance of the region with extremely low reflection of electromagnetic waves, i.e. antireflective channel formation in the far and middle IR range is associated with the resonant interaction of wave with crystal polar oscillations. Minimum reflection can be reduced by several orders compared with non-resonant regions, almost to complete the reflection disappearance ($R < 0.01\%$). The main feature of zero-reflection is frequency shift of ARC relatively to T-L frequencies beyond the existence limits of negative dielectric permittivity.

STRUCTURE OF LAYERED MIXED CRYSTALS ON THE BASED PBI$_2$

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The I^{127} Nuclear Quadrupole Resonance (NQR) spectra of the mixed semi conducting laired crystals BiI$_3 \cdot$PbI$_2$ for two transitions ($\pm 1/2 \leftrightarrow \pm 3/2$ and $\pm 3/2 \leftrightarrow \pm 5/2$) were investigated.

It was obtained, that for the chemically pure crystals BiI$_3$ the I^{127} NQR frequencies υ, which correspond to two transitions ($\upsilon_{\pm 1/2 \leftrightarrow \pm 3/2}$ and $\upsilon_{\pm 3/2 \leftrightarrow \pm 5/2}$), equal to 111.320 and 201.380 MHz. This leads to the next values of the I^{127} NQR spectra parameters: the quadrupole coupling constant $e^2Q_{zz} = 682.18$ MHz and the parameter of asymmetry of the electric field gradient $\eta = 29$ %.

In the first time the new I^{127} NQR line in spectra mixed crystal was observed in the concentration region 10 - 50 %. It is necessary to note, that for this concentration region the I^{127} NQR line, which correspond to the chemically pure crystals BiI$_3$, became invisible. The new observed I^{127} NQR line has the next parameters: $\upsilon_{\pm 1/2 \leftrightarrow \pm 3/2} = 105.027$ and $\upsilon_{\pm 3/2 \leftrightarrow \pm 5/2} = 204.150$ Mc^{-1}, $e^2Q_{zz} = 684.01$ Mc^{-1} and $\eta = 15$ %. In the concentration range 20 -50 % the wide of the I^{127} NQR line (2.1 – 2.3 Mc^{-1}), which correspond to transition $\pm 3/2 \leftrightarrow \pm 5/2$, changes insignificantly.

The obtained results allow make suppose, that in the concentration region 5 -10 % the crystal structure of the base crystal BiI$_3$ changes insignificantly. Moreover, in this concentration region 5 -10 % the arising of the clusters PbI$_2$ does not change (insignificantly) wide of lines and parameters of the I^{127} NQR spectra. Besides, for the concentration PbI$_2$ more then 10 % in the base matrix BiI$_3$, can be obtained a new crystal with fully or partial ordering groups of atoms Pb and Bi. This can lead to the formatting of the new crystal of the solid solution type and, as result, to sharp changing of the I^{127} NQR parameters values.

For checking this assumptions it is necessary camper the obtained NQR data with experimental results, obtained by another methods (for instance by X-ray investigations).

ALKYL CHAIN CONFORMATION AND PHASE TRANSITIONS IN COMPLEXES OF FATTY ACID WITH CATIONIC SURFACTANT

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Complexes of amphiphilic molecules of fatty acids with cationic surfactant may be useful for fabrication of self-assembled non-centrosymmetric organic layers by evaporation induced precipitation method [1] for applications in molecular electronic devices. In this work we report on the study of the alkyl chain conformation and molecular dynamics in complexes consisting of a fatty acid and water soluble cetyltrimethyl ammonium bromide ($C_{19}H_{42}NBr$, CTAB).

The complexes of stearic ($C_{17}H_{35}COOH$, k18) and behenic ($C_{21}H_{43}COOH$, k22) acids with CTAB were characterized by X-ray diffraction, temperature-dependent Fourier-transform IR spectroscopy (FTIR) and differential scanning calorimetry (DSC). X-ray diffraction patterns (DRON-2) show that in the both complexes a layered crystalline structure is formed. The interlayer distances of CTAB and k22 are close and these results in a formation of CTAB-k22 complex with similar distance between the layers. This suggests that alkyl chain orientation and crystalline packing in the complex are close to those in initial substances. To the contrary, a significant difference between the interlayer distances of CTAB and k18 crystals exists, and therefore the interlayer distance observed in CTAB-k18 complex differs much from that of the both initial compounds. So, the alkyl chain packing and orientation in CTAB-k18 complex may be changed as compared to the initial crystals. DSC studies (Perkin-Elmer DSC7) of the both complexes reveal the existence of two major endothermic peaks at the temperatures close to the second-order phase transitions in the initial compounds, though the enthalpies of these transitions differ from the initial ones. The FTIR absorption spectra (Bruker IFS-88, 2cm^{-1} resolution, 64 scans) of CTAB-k18 and CTAB-k22

complexes show that the carbonyl band (1710 cm^{-1}) of pure acid disappears in the spectra of both complexes that confirms the attachment of CTAB head group to the OH group of the acid and formation of CTAB-acid complex. From the temperature dependence of the Davydov splitting of CH$_2$ rocking (720-730 cm^{-1}) and scissoring (1460-1470 cm^{-1}) absorption bands, the changes of alkyl chains packing at phase transitions in different complexes are inferred.

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INFLUENCE OF A PROTON IRRADIATION ON THE MECHANISM TEMPERATURE SUPPRESSIONS LUMINESCENCE OF CERAMICS ZNS-CU

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By interaction of the center's of capture and centers of a luminescence, is determining kinetic luminescence in solid-state luminescent materials. At an irradiation there is a change of the contents of impurity and defects that result in change of optical properties of a crystal.

Influence of stable radiating defects entered by a proton irradiation (10^{15} p/sm^2) on temperature quenching of a luminescence of ceramics ZnS-Cu was studied. The spectra of X-ray luminescence (XRL) at temperature 85K for the irradiated and not irradiated ceramics are observed three bands: blue band (λ_{max} = 465 nm), green band (λ_{max} = 520 nm) and the infrared band (λ_{max} = 942 nm). Comparison of data XRL, to a phosphorescence and termostimulated luminescence (TSL) of ZnS from a dozen of proton irradiation has shown that generated radiating defects do not create the new centers of a luminescence or storage, and behave as the centers of nonradioactive recombination. The received results were analyzed on the basis kinetic of the theory photoluminescence crystallophosphor, in view of absorption of stimulating radiation in the basic lattice.

Experimental temperature researches were carried out in region from 85 up to 600K. Temperature dependences of a luminescence blue and infrared have not changed after a proton irradiation. The temperature quenching of a blue band begins at T=170K and infrared band at T=150K. For a green band of a luminescence in the irradiated sample typically: decreasing of intensity of a stationary luminescence and beginning change of the temperature quenching in low temperatures. Is determined energy of thermal activation of temperature quenching of a luminescence. On the basis of the received data on temperature quenching and curves TSL for both samples, it is possible to assume, that as against blue and infrared bands, quenching of a green band is caused by outward quenching (thermal ionization of recombination center). Charge double vacancy of zinc give is one of prevailing types of defects and enters into structure of the «green» centers Cu. At a used doze the proton irradiation to be result accumulation of radiating defects; the green strip can almost be completely extinguished at warm of samples in pairs of zinc.

The radiating defects, induced by a proton irradiation, result in change kinetics of luminescent processes and testify to change of a spectrum of local statuses in a researched material.

CHIRAL CALIXARENES: STRUCTURE AND OPTICAL PROPERTIES

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Calixarenes are widely used in supramolecular chemistry. Because of their chalice shape calixarenes easy make complexes with other molecules. This fact makes these compounds suitable for molecular receptors, sensors, catalysts, molecular separations, etc. The addition of chirality to calixarenes gives them an important role for enantioselective separations and receptors, nonlinear optical components, chiral catalysts and so on.

We have recently synthesized and investigated the enantiomers of 5,11,17,23-tetra-tert-butyl-25-hydroxy-26,27-dipropyloxy-28-N-(1›-phenylethyl)aminocarbonylmethoxycalix[4]arene.

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

The optical properties of the calixarenes have been studied. The optical activity confirmed the chiral nature of substances. Raman spectra of calixarenes in solid state and solution were measured to analyse the vibrational structure of the compounds.

PHONONIC AND MAGNETIC EXCITATIONS IN THE QUASI-ONE DIMENSIONAL HEISENBERG ANTIFERROMAGNET KCUF$_3$

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The system KCuF$_3$ is a good realization of one-dimensional spin-1/2 Heisenberg antiferromagnet [1,2]. This compound realizes an array of weakly coupled spin chains in high-temperature regime whereas long-range A-type antiferromagnetic ordering occurs below T_N=39 K. To date, even the room temperature crystal structure of KCuF$_3$ seems not to be determined unambiguously. Recently, the ESR and optical properties of KCuF$_3$ were successfully explained within the tetragonal symmetry D_{4h}^{18} assuming a dynamical Dzyaloshinsky-Moriya interaction related to strong oscillations of the bridging F$^-$ ions perpendicular to the crystallographic *c* axis [3,4]. It was argued that these dynamic distortions freeze in at a temperature T_S = 50 K, leading to an effectively lower symmetry.

Here we report on a detailed study of the temperature dependence of the Raman-active phonons in a KCuF$_3$ single crystal tracking the symmetry reduction during the anticipated freezing of the dynamic distortion at T_S=50 K and the Neel ordering at T_N=39 K and a complete data set of the magnetic excitations in this compound collected for the first time by using Raman scattering experiment.

We find a large softening of the lowest lying E_g mode and the B_{1g} mode by 25% and 13% between room temperature and T_S, respectively. The linewidth and the integrated intensity of these modes also exhibit anomalies at T_S and T_N. Moreover, the E_g mode at about 260 cm^{-1} clearly splits below T_S evidencing a symmetry reduction in KCuF$_3$ at T_S=50 K prior to magnetic ordering.

At $T < T_N$ magnetic excitations characteristic of 3D and 1D magnet were observed in our Raman experiment. The energy ranges of these phases are separated by another region where the crossover from 1D to 3D behavior occurs.

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INFLUENCE OF POLYMORPHISM AND HYDROGEN BONDING ON VIBRATIONAL SPECTRA OF CYCLOHEXANOL

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Vibrational spectra of cyclohexanol in liquid state and at different polymorphous modifications II, III have been measured in wide temperature range. Pilot analysis of spectra indicates formation of hydrogen bonds. Spectra of polymorphous modifications differ from each other by the packing which subject to hydrogen bond influence and prevalence of selected conformers. Using B3LYP/6-31G (d) method structural - dynamic models of conformers of cyclohexanol molecule and its H-complexes (trimer, tetramer) have been constructed. The conformers of cyclohexanol differ from each other by orientation of hydroxyl group and types of H-complexes. The energy minimization, structure optimization, dipole moments have been performed. The force field was built and the frequencies of the normal modes in harmonic approximation and IR intensities have been calculated. On the basis of simulated results the correspondence between the H-complexes structures of different conformers and polymorphous modifications have been determined. The interpretation of the measured spectra has been performed.

INVESTIGATION OF VIBRATION SPECTRUM OF FERROBORATE TBFE$_3$(BO$_3$)$_4$

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Trigonal rare-earth borates with the general formula $RM_3(BO_3)_4$, where R is a rare-earth ion and M=Al, Ga, Sc, Cr, and Fe, are of interest as laser materials and materials which can be used in magneto-optical devices. The ferroborate family $RFe_3(BO_3)_4$ is interesting due to the particulars of the formation of their magnetic structure, which is determined by the interaction of rare-earth ions with iron ions. The magnetic properties of ferroborates also depend on the rare-earth ion. The strong spin-orbit coupling in rare-earth ions should lead to an interaction of magnetic excitations and vibrations of the crystal lattice. The coupling of the magnetic excitations and IR active vibrational modes determines the magneto-electric properties of these materials. Ferroborates, where this coupling is quite strong, are multiferroics [1]. To determine the magnitudes and mechanisms of the magnetoelectric coupling it is necessary to know the structure of the IR active vibrational spectrum of crystals and the mechanism by which it forms. In the present work the IR active vibrational spectra of one of the members of the series of rare-earth ferroborates—the $TbFe_3(BO_3)_4$ crystal—are investigated

The investigated single crystal was cut in the form of a 1×4×5 mm plate which surface was perpendicular to the trigonal axis *c*. The IR reflection spectra of a $TbFe_3(BO_3)_4$ crystal are measured in the spectral range 200–2000 cm^{-1} in E perpendicular to *c* axis polarization at temperatures 10 and 300 K. The reflection spectrum so obtained is analyzed and its interpretation is given on the basis of the internal vibrations of the ionic complexes BO_3^{3-}, FeO_6^{9-}, and TbO_6^{9-} of the $TbFe_3(BO_3)_4$ crystal. Davydov splitting on the internal vibrational modes at a structural phase transition which is accompanied by multiplication of the unit cell was not observed in the experimental spectral range. This is due to the localization of the vibrations of the ionic complexes BO_3^{3-}, FeO_6^{9-}, and TbO_6^{9-} of the $TbFe_3(BO_3)_4$ which defines by the crystal structure of $TbFe_3(BO_3)_4$.

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OPTICAL DETECTION OF RADIATION-INDUCED DEFECT PHASE FORMATION IN XENON CRYOCRYSTALS

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Among various material processing techniques the radiation technology of crystal structure modification by low-energy irradiation is one of the most agile manufacturing method. Xenon cryocrystals are widely used as the model systems in fundamental investigations of electronically induced lattice modification and as the working media of particle detectors and positron moderators. The electronic excitations in solid Xe have been under investigation since seventies and now the overall picture of creation and trapping of electronic excitations is basically complete [1]. The spectroscopic properties of radiation-induced processes in solid Xe under synchrotron irradiation (at HASYLAB, DESY, Germany) were well studied recently [2]. In the present study we apply the kinetics methods for numerical simulation of defect processes in irradiated crystals and harness the rich luminescence spectra of solid Xe for real-time monitoring of their crystal structure.

Initial increase of the intensity of the 'defect' luminescence during irradiation reflects the accumulation of Frenkel pairs in the lattice as a result of exciton creation and self-trapping in the consecutive process $E + T \leftrightarrow MTE \rightarrow D$, where E is the mobile excitation (free exciton), which is trapped at trapping center T (lattice imperfection) and forms an excited metastable trapped center MTE [3]. The time dependence of 'defect' luminescence intensity under steady-state conditions is: $I(t) = I_0 + K \cdot t \cdot (L + t)^{-1}$, where $I_0 = I(0)$ is the initial intensity; K is the saturation value of $(I(t) - I_0)$ at $t \rightarrow \infty$; $L \sim n_E n_T (n_{MTE})^{-1}$ is a characteristic constant of a sample, n – concentration. At high defect concentration, n_D, the exciton self-trapping near existing defects induces the aggregation of defects in the process $MTE + D \rightarrow DD$. The time dependence in this case is $I(t) = K \cdot L' \cdot (L' + t)^{-1}$, where $L' \sim n_{MTE} n_D (n_{DD})^{-1}$. The best fit of our data for solid Xe results in values $K = 1668$ cps, $L = 43$ min, $L' = 814$ min. Thus, optical detection of radiation-induced new defect phase formation in xenon cryocrystals was made by luminescence-kinetic method.

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NEW APPROACH FOR STUDY OPTICAL PROPERTIES OF PHOTONIC CRYSTALS

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Synthetic opal is a structure consisting of densely packed silica near-monosize globules of diameter that is close to wavelength of visible light. Essential interest to opals is connected with their application as photonic crystals (PC) [1,2].

The properties of PC are studied in visible region, mainly in the region of 1-st and 2-nd orders of Bragg diffraction. Typically, the materials with index of refraction close to those in PC globules are introduced into the cavity of PC for transmission measurements. It is necessary to decrease the diffuse scattering of light by PC. Total scattering of PC (λ=632,8nm) at normal incidence is equaled to 88% (for the PC of good quality) and could reach 99% for PC with numerous defects. Bragg scattering intensity reaches 1-12%. This means that diffusion scattering is in the 80-90% range.

To characterize the molecular vibrations of PC and impurities in the pores we have used the IR spectroscopy. Thick PC (with thickness 1-3 mm) without substrates demonstrates an insufficient transmitted signal in the infrared spectral range due to intense light scattering. Under IR reflection spectra registration of PC on the absorbing substrate (black paper), the reflected signals from silica stretching ($1120 cm^{-1}$) and deformation ($450 cm^{-1}$) vibrations is very low. We proposed to use the thin film gold support for PC during IR reflection measurements. This approach gives a possibility to register the vibrations of SiO_2 accurately as well as different defects and admixtures in PC, namely Si-O-H, OH vibrational modes, H_2O dynamics in PC.

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SPECTROSCOPY OF IMPURITY STATES IN CU-MN ALLOYS

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The results of measurements of optical and electronic properties of disordered Cu-Mn alloys with manganese concentrations of 2, 5, 10, 17.5, 25, 37.5 and 50 % are presented. The indices of refraction n and absorption χ of disordered Cu-Mn alloys are measured in the wide spectral range 0,23-2,8µm (0,44-5,39 eV) at room temperature using the spectroscopic ellipsometric technique. Based on these data, the optical conductivity σ related to interband transitions is calculated. The collision frequency γ and the concentration of conduction electrons N are determined in the interband absorption region.

It is established that an impurity of antiferromagnetic manganese added to copper results in the in the formation of a new impurity energy band in the copper electron spectrum which is located approximately 2.2 eV lower than the Fermi level and is split into two energy subbands due to the exchange interaction.

It is shown that the electron spectra of Cu-Mn alloys represent a superposition of the electron state densities $g(E)$ of pure copper with a certain weight equal to the manganese concentration in the alloy and the state density within the impurity band. It is shown, that interband transitions from the *d*-bands of the solvent to its *sp*-bands result in the formation of fundamental absorption bands $\sigma(hv)$ in Cu-Mn spectra. Additional bands appear due to electron transitions from the impurity band to the Fermi level E_{F}.

Key words: alloys of copper with manganese, impurity band, energy subzone, frequency of collisions, concentration of electrons, interband junction, intraband junction, density of electronic state, optical conductivity spectrum.

PHOSPHORESCENCE OF TWO POLYMORPHS OF PARA-BROMBENZOPHENONE

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Phosphorescence spectra of two polymorphs of para-brombenzophenone (4BrBP) were measured at two temperatures 1.6 K and 293 K. The stable polymorph has a monoclinic structure ($P2_1/c$, $Z = 4$) while the metastable one is triclinic ($P1$, $Z = 2$). The stable phase was obtained by gradient sublimation, and the metastable phase by Bridgman method [1].

Both polymorphs have a monomeric spectrum which resembles that of benzophenone. Phosphorescence spectra of both polymorphs have vibrational bands (the C=O stretch mode, the separation between bands ≈ 1680 cm^{-1}), each of which has contains narrow subbands due to exciton emission on traps. The exciton bands in the two polymorphs are shifted to one another. This gives evidence that the energy positions of the exciton bands in the polymorphs differ. Theoretical calculations corroborate this conclusion.

The room-temperature phosphorescence spectra are also monomeric, the bands being broadened compared to low temperatures.

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CRYSTAL GROWTH OF THE 2-ACETYLDIMEDONE BORIC CHELATE MEROCYANINE DYES UNDER DIFFERENT CONDITIONS: MOLECULAR STRUCTURE AND OPTICAL PROPERTIES

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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" (ca. 0.06 x 0.06 to 0.15 x 0.15 mm in section). The using of solvents such as acetonitrile causes the growth of classic single crystals. With the imposition of the external electro-magnetic field 750 kV/m (with using any solvent type) all crystals have a classic form, but they become thinner and notably longer than without the field.

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.

NATURE OF CRYSTALS LUMINESCENCE UNDER ULTRASONIC EXCITATION

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The assumption of the common nature of an acoustical luminescence (luminescence of solids at excitation by ultrasound) [1] and sonoluminescence of liquids [2] was made in this report. The main idea is that the microcracks in crystals are the solid-state analogues of cavitation bubbles in liquids. Such microcracks are originated and vanished in result of ultrasound action. Appearance of microcracks can be accompanied by various processes, which are the reasons of excitation of luminescent centers.

Investigated monocrystals of zinc sulphide were grown from the melt by the Bridgman method under pressure of inert gas. Concentration of manganese in crystals was $5*10^{-4}$ %. Elastic deformation on the samples was directed along the $[111]_c$ axis. Ultrasonic vibrations which were produced by piezoelectric ceramic transducer were directed perpendicular to the $(1\bar{1}0)$ plane. For easier origination of microcracks, ultrasonic oscillations were applied to crystals together with constant elastic loading, as displacement. The amplitude of ultrasonic oscillations applied to the crystal did not change. Constant mechanical displacement gradually was increasing until destruction of crystal.

Registration of radiation in ZnS crystals was carried out continuously on the wave length $\lambda = 585$ nm. This magnitude corresponds to the maximums of all luminescence types namely photo-, electro-, tribo- and luminescence which was observed during mechanical destruction of the investigated crystals.

Joint action of the constant amplitude ultrasonic vibrations and static uniaxial compression was supposed to create a situation where the total magnitude of the variable and constant load reaches the value necessary for the appearance of microcracks. It was found that under static pressure of $P = \sim 20*10^7$ Pa the samples begin to emit radiation on a wavelength $\lambda = 585$ nm. Intensity of this radiation is increasing with time. After some period of time (5-7 sec) the samples are breaking with splash of light emission which rapidly decreases.

The results confirm the assumption that the luminescence being caused by action of acoustic oscillations on the crystals is associated with processes caused by the appearance and "healing" of microcracks.

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MULTIPLET STRUCTURE OF THE LUMINESCENCE SPECTRA OF THE DOPED MOLECULAR CRYSTALS

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The luminescence and absorption spectra character for a series of organic molecules incorporated to the different matrixes (crystal-solvents) at low temperatures is related to the different types of incorporation of the doped molecules to the matrix.

The luminescence spectra of the monosubstituted molecules of naphthalene and benzophenone which are incorporated to naphthalene and benzophenone crystals as a matrix are characterized by a doublet structure due to the emission from the independent sites.

Based of the symmetry of a free naphthalene molecule, impurity and naphthalene crystal, the number impurity centre formed in naphthalene crystals with impurities of naphthalene substituents is determined. It has been established that the origin of the multiplets in the Shpolsky spectra and molecular impurity crystals for some impurities is the same.

ELECTRONIC STRUCTURE OF LUMINESCENCE PROPERTIES OF DOPED WITH CR AND NI IONS ZINC AND CADMIUM TUNGSTATE CRYSTALS

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It is generally accepted that presence of non-luminescent non-neutral impurities strongly affect the luminescence properties of zinc and cadmium tungstates. However, the mechanism of this influence is not well understood. In this work we study both pure $ZnWO_4$ and $CdWO_4$ and doped with Cr^{3+} and Ni^{3+} ions at various concentrations by experimental spectroscopy under the VUV synchrotron and visible laser excitations together with theoretical calculations of the electronic structure. Monoclinic tungstates of divalent ions like Zn^{2+}, Cd^{2+} are host lattices suitable to accommodate Cr3+ ions in weak field octahedral sites..   Only $ZnWO_4$:Cr has been studied in some detail, whereas the information concerning other doped similar materials is dated and incomplete.

Pure and doped single-crystalline samples were synthesized by the Czhochralski method. The VUV-excited luminescence properties were studied in 3.5–20 eV regions of excitations energies on SUPERLUMI station (synchrotron laboratory HASYLAB (DESY) Hamburg, Germany). Crystals obtained at 8 K and 300K consist of the band in 350 – 1000 spectral region with maxima at about 500 and 560 nm at different excitations (90- 300 nm). For the doped $Zn(Cd)WO_4$ crystals these maximums are 500, 560 nm and 950 nm at the same excitations.

The electronic structures of perfect and impure crystals were calculated using full-potential linear-augmented-plane-wave (FLAPW) method [1].

Experimental data are analyzed along with results of theoretical calculations. The role of impurities Cr^{3+} and Ni^{3+} in formation of the spectroscopic properties of zinc and cadmium tungstate crystals is elucidated. General inferences concerning participation of defects in formation of the luminescence spectra and other spectroscopic properties of tungstate crystals are made.

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EVIDENCE OF ANOMALOUS POLARITONIC LUMINESCENCE FROM SOLID XE

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The exciton-photon interaction leads to the formation of polaritonic states energetically positioned at both sides of the initial exciton. In a large ideal crystal of cubic symmetry, where the interval of the longitudinal-transverse splitting does not contain excitonic levels, the polaritonic dispersion branches lie beyond this interval at both sides of its boundaries. On the contrary, in a crystalline grain comparable or less in size than the wavelength in the substance, the interval of the longitudinal-transverse splitting is filled in continuously by excitonic states intercepting a significant part of the oscillator strength of the excitonic transition. In the previous experiments with polycrystalline samples of solid xenon the formation of the lower polaritonic state was traced by the red shift of the luminescence spectrum relative to the bottom E_1=8.36 eV of the lowest excitonic band [1].

In the present paper we explore the new crystal growing technique, which allowed to obtain the solid Xe samples with essentially improved crystallographic properties [2] and to resolve the internal structure of the luminescence bands at the edge of exciton absorption [3]. The photoluminescence experiments were carried out at the SUPERLUMI experimental station at HASYLAB, DESY, Hamburg. Unlike previous works, where the observed red polaritonic shift was small commensurably with a weak inelastic polariton-photon scattering, a large polaritonic shift of luminescence is not due to energy dissipation, the energy conservation law being met due to equal probabilities for opposite-sign energy shifts. Such effect is possible if the crystalline grains are comparable in size with light wavelength, which provides the filling in the interval of the longitudinal-transverse splitting by excitons with sufficient oscillator strength. And the sample structure must be perfect enough to lowering the exciton scattering rate with respect to the rate of the polariton formation through exciton-photon coupling. For the first time the excitation spectra of free-exciton luminescence band were recorded simultaneously below E_1 and within the interval of the longitudinal-transverse splitting. The luminescence

of non-equilibrium polaritons was observed both within the longitudinal-transverse splitting interval and at photoexcitation below the bottom of the excitonic band.

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AGAIN ABOUT THE NATURE OF NON ELEMENTARY BANDS OF MN2+ LUMINESCENCES SPECTRUM IN ZNS

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There are many questions about the number and the nature of the elementary bands in luminescences spectrum of Mn2+ in ZnS crystals during long time. In the connection with unique opportunity to obtain the crystals with any structure from 3C to 2H, in this article the trying of the exact identification of some elementary bands of manganese photoluminescence in ZnS crystals was made.

The relation of different types MnZn2 + centres in the research samples was determined by ESR measurements. If each of these types of centres take part in formation of a common band of a Mn2+ luminescence, then by means of corresponding mathematical processing of spectroscopic lines probably their partitioning and the further exact identification. It main idea of our experiments which was realized here.

As have shown our experiments, this idea was correct. Really, at controllable change of quantity of various sites in structure of crystals, we managed to see changes in spectrum PhL. It has helped to find out connection of some elementary components of a spectrum with concrete places of localization of the centers of manganese in a crystal lattice.
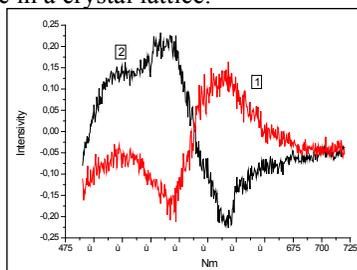
Fig. 1. (1) - result of subtraction of original spectrum from the spectrum heat treatment 800C ; (2) – result of subtraction of the spectrum heat treatment 800C from the spectrum heat treatment 1100C.

According to the characteristic of the picture here it is seen the change of elementary bands of manganese photoluminescence in ZnS crystals. This is discussed in this report.

PHOTOLUMINESCENCE AND ESR IN THE LINAGE$_4$O$_9$ CRYSTALS DOPED BY MANGANESE

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The Photoluminescence and ESR-spectrums of manganese impurity ions in LiNaGe4O$_9$ crystals, growth by Chohralski method were studied in this work. It is known, that crystals of LiNaGe$_4$O$_9$, are in a paraelectric phase and has orthorhombic lattice cell (Pcca - D82h) at room temperature. The transition to ferroelectric phase takes place at the temperature Tc = 112,7 K.

It was discovered, that at T = 300 K in studied crystals, the ESR-spectrums in X-range consist of three intensive groups of hyperfine structure (HFS) lines, each of which is conditioned by ions of manganese, in some almost identical positions with orthorhombic local symmetry.

The main values of the g-factors are obtained: g_{xx} = 1,7444, g_{yy} = 2,2948, g_{zz} = 2,5631. The hyperfine structure constants of all spectrums have a strong anisotropy. It was discovered, that the local symmetry of manganese paramagnetic centers and the parameters of their ESR-spectrums are not changing, when the temperature of crystals are decreasing to magnitude corresponding phase transition to ferroelectric phase.

But ESR dates was not enough for answer on the main question about charge state Mn ions. That is why was decided to investigate the photoluminescence properties in these crystals. As was found there are two maximums in luminescence excitation spectra on 392 nm and 472 nm (77K).

Spectra of luminescence has one complicated band with maximum on 665-680 nm when wave-length of excitation is 472 nm. It is very similar that this band of luminescence correspond to transition 2E → 4A for Mn^{4+} ions. But when wave-length of excitation is 392 nm, the spectra of luminescence has two bands. One of them is the same as the wave-length of excitation was 392 nm.

Another band of luminescence with maximum on 550 nm, may be caused by 5E → 5T2 transition in ions of Mn^{3+}. It is important note, that Mn^{3+} ions by ESR method not observe.

In addition to results about charge state and local symmetry of Mn ions was determine frequencies of lattice vibration by periodic luminescence maximums on wings of spectra lines.

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

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Low-temperature thermal and magnetic-resonance studies show that in monoclinic KDy(WO$_4$)$_2$ single crystal a structural phase transition (SPT) at 6.38 K takes place. The magnetic field dependence of the critical temperature is observed. The prominent features of the SPT are typical for a second-order Jahn-Teller transition, which is not accompanied by any change in the symmetry of the crystal lattice in the low-temperature phase [1]. A steplike irreversible variation in the elastic strain is observed to occur with an increase in the magnetic field applied along the *a* or *b* axis of the crystal monoclinic cell. This variation disappears after thermal cycling at temperatures which are essentially higher than SPT one [2].

This compound was studied earlier by Raman scattering method [3]. A number of additional spectroscopic studies at different temperatures and in external magnetic field were performed in order to explain new unusual effects observed in KDy(WO$_4$)$_2$.

Spectrum of the Raman light scattering is investigated in KDy(WO$_4$)$_2$ single crystal in the frequency range 3–950 cm^{-1} in the temperature range 2–300 K. All 36 vibrational modes predicted by group theory analysis for high-temperature phase were detected and their symmetries were determined.

It is established that first excited electronic quasi-degenerated doublet is splited higher SPT temperature (6.38 K), and at lower temperatures has complicated structure, containing in scattering spectrum four lines. This fact indicates the presence of four nonequivalent ions of dysprosium in low temperature phase.

Creation of three additional phonon lines, which indicates primitive translation cell doubling at phase transition, is observed in low temperature phase at 2K.

The measurements in magnetic field have shows that scattering spectrum transformation on first exited electronic quasi-doublet takes place. This transformation indicates on the presence of phase transition induced by magnetic field.

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SPECTROSCOPIC AND MAGNETOOPTICAL INVESTIGATIONS OF MAGNETIC INTERMEDIATE STATE IN TBFE$_3$(BO$_3$)$_4$ SINGLE CRYSTAL

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As known from the magnetometric measurements [1], spin-orientation phase transition occurs in antiferromagnetic TbFe$_3$(BO$_3$)$_4$ at $\boldsymbol{H} \parallel C_3$ ($H_c = 35$ kOe at $T = 4.2$ K). We performed spectroscopic and magnetooptical investigations of this crystal to clarify the peculiarities of the transition.

Optical absorption spectra of single crystal TbFe$_3$(BO$_3$)$_4$ were studied in the region of $^7F_6 \rightarrow {}^5D_4$ transition in Tb^{3+} ion in external magnetic field $\boldsymbol{H} \parallel C_3$ (0 – 60 kOe). At $H < H_c$ the absorption lines undergo linear in the field strength splitting, conditioned by nonequivalence of magnetic sublattices. Measured splitting of the absorption lines in magnetic field permitted us to obtain the corresponding splitting of states and their Landé factors.

In the region of the phase transition a superposition of the spectra of low-field and high-field magnetic phases is observed. It testifies to the existence of a magnetic intermediate state with the periodic alternation of domains of the both magnetic phases. In the same interval of magnetic fields the considerable reduction of light transmission of the crystal is observed, which is a consequence of strong light scattering arising in the region of the phase transition.

Visual polarization investigations of the domain structure of the magnetic intermediate state were performed. It was shown that the high-field magnetic phase arises as cylindrical domains which are transformed into a labyrinth domain structure with the increasing field. The strong scattering of light by the crystal is the result of the magnetic two-phase domain structure. The measurements of Faraday rotation and magnetic linear birefringence at $\boldsymbol{H} \parallel \boldsymbol{k} \parallel C_3$ were performed. In the high-field magnetic phase the large magnetic circular birefringence appears. Its value is an order of magnitude larger than the value of the linear birefringence. This allows us to infer that the main mechanism of the light scattering on the domains is related to the large value of the Faraday rotation in the high-field magnetic phase domains.

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TEMPERATURE DEPENDENCE OF LOW-FREQUENCY RAMAN SPECTRUM OF CRYSTALLINE 2-(2'-HYDROXYPHENYL)BENZOXAZOLE

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2-(2'-hydroxyphenyl)benzoxazole (HBO) is a photoluminescent material emitting in the green spectral region with a maximum of an emission band at 506 nm. Its bright fluorescence with a quantum yield of about 0.42 in the crystalline state is caused by tautomeric species of HBO molecules formed by the excited state intramolecular proton transfer. After photoexcitation large amplitude twisting of the molecule in the excited state is supposed to be responsible for a radiationless deactivation process decreasing the quantum yield of the luminescence down to a value of about 0.018 in solution at room temperature [1].

Non-polarized Raman spectra in the frequency region 15-250 cm^{-1} of the HBO single crystal have been studied in the temperature range 293-393 K. The Raman spectrum comprises two narrow very intense bands in the region 15-50 cm^{-1}, five strong bands of approximately equal intensity in the region 50-130 cm^{-1}, two medium and one weak wide bands in the region 130-250 cm^{-1}. The parameters of 12 vibrations have been obtained by fitting of the observed spectra with the use of the model of weakly interacting oscillators.

A crystal of HBO belongs to the structure class Pna2$_1$ with 4 molecules per unit cell [2] so that, under the rigid body approximation, 21 intermolecular vibrations are expected to be active in Raman spectrum and strict separation of translational and librational modes is not possible. The density functional theory (DFT) calculations performed for an isolated molecule of HBO show its flexibility and predict 5 internal vibrations below 250 cm^{-1} at 58, 66, 116, 164 and 244 cm^{-1} (unscaled values).

The temperature dependence of the spectra does not demonstrate preferable disappearance of any Raman bands in the region studied. It may be concluded that reorientation of the molecules is hampered by crystal packing.

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THE ROLE OF WEAK INTERACTIONS IN THE FORMATION OF SUPRAMOLECULAR STRUCTURES OF BORONIC ACIDS

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Boronic acids $RB(OH)_2$ are the compounds able to take part in various supramolecular systems due to the presence of different reactive centres in one molecule. Two hydroxyl group can be involved in various homomeric and heteromeric hydrogen-bonded assemblies [1], as well as in condensation reaction leading to covalently bonded systems, e.g. the esters with hydroxyl compounds [2,3]. The dehydration products, boroxins, are the promising building blocks in the design of molecular architectures and materials [4]. Lewis acidic character of the boron atom makes possible the complex formation with Lewis bases, e.g. anions.

Flexibility of the boronic acid molecule plays the important role in the diversity of the systems. The presence of two hydroxyl groups in different conformations (Fig. 1) enables the formation of hydrogen bonded assemblies in one-component systems (only boronic acids) or multi-component ones [1].
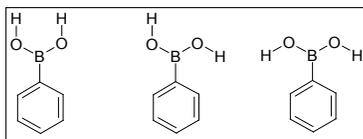
The properties of boron compounds result not only from the boronic groups, but also from weak interactions with other parts of the molecule. Hence, the investigations of the supramolecular structure of substituted boronic acids may be of significance.

Several examples of the influence of the substituents in the phenyl ring of phenylboronic acids on the higher supramolecular levels will be presented, including isomers of formylphenylboronic acids and fluoro-substituted phenylboronic acids. The Hirshfeld surface analysis will be applied as the useful tool for depicting types and directionality of weak intermolecular interactions [5].

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PYROELECTRIC EFFECT IN THE POLYDOMAIN TRIGLYCINE SULFATE CRYSTAL

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Existence of domains essentially influences all characteristics of ferroelectric materials, first of all on their electrophysical properties. Especially it is shown at research of character of the response of a ferroelectric material in the process of absorption of radiation at pyroelectric effect. It was observed in experimental works, research of characteristics which cause this influence, and creation of adequate theoretical models of these processes however wasn't offered.

Modern sections of physics of ferroelectric phenomena demand not only understanding of processes of domain structure construction in a ferroelectric material, but also developments of experimental methods of research of evolution of this structure and the mathematical description of these processes.

The purpose of this work consisted in experimental and theoretical research of influence of domain structure and its evolution on temperature characteristics of a signal of the pyroelectric response in the ferroelectric triglycine sulfate crystal (TGS).

Measurement of a signal of pyroelectric response U of the experimental sample on action of laser radiation (P = 3mW) was carried out in the pyro-EMF mode at dynamic pyroelectric effect. The obtained experimental results have shown essentially not monotone character of temperature dependence U (T).

Experimental features of the spent researches consisted in use of a laser probe for control of parameters of domain border movement in the process of the crystal temperature change from the room temperature to the Curie temperature $T_C = 49^0C$. Speed of crystal temperature change in the process of measurement was the 1^0C/minute. Values of displacement of domain walls have been measured from initial position at room temperature to their positions in process of change of temperature approach to Curie temperature, and these measurements were spent at temperature change through each 5^0C. Values of displacement of domain borders were

measured by means of a laser probe which had the diameter size d = 20μm.

The obtained experimental results of temperature dependence of domain walls displacement have been used for creation of phenomenological model of pyroelectric response of the TGS crystal on action of laser radiation.

On the basis of the spent researches temperature dependences of the unipolarity coefficient η (t) and the pyroelectric response signal U (T) of polydomain ferroelectric material have been theoretically obtained. It is shown that a local maximum of curve

U (T) correspond to a maximum on curve of temperature dependence of domain borders displacements.

The obtained theoretical results of research of influence of domain structure evolution on pyroelectric response of the TGS crystal quantitatively describe experiment.

INVESTIGATION OF MAGNETIC PHASE TRANSITION IN TBFE$_3$(BO$_3$)$_4$ SINGLE CRYSTAL BY RAMAN SCATTERING

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Compound TbFe$_3$(BO$_3$)$_4$ undergoes a structural phase transition at 198 K and magnetic ordering transition at about 40 K. The nuclear and the magnetic structure of TbFe$_3$(BO$_3$)$_4$ as a function of temperature were determined using neutron diffraction measurement [1]. Recently, the Raman spectra of the compounds RFe$_3$(BO$_3$)$_4$ with R = Gd, Tb, Er, and Y were measured in Ref. [2] as a function temperature. In present report the results of investigation of vibrational and magnetic excitations in TbFe$_3$(BO$_3$)$_4$ crystal in temperature range of the magnetic transition and their behavior in an external magnetic field are presented.

The Raman scattering spectra on compound TbFe$_3$(BO$_3$)$_4$ were investigated in the frequency range 3-500 cm^{-1} at temperatures 2-300 K. The measurements were carried out on single crystal oriented along the C$_3$ and hexagonal axes of the trigonal phase.

A number of additional phonon lines in comparison with Ref.2 were observed above and below the structural phase transition. These lines are the result of LO –TO splitting of polar phonons in high-temperature phase. New data from the Raman spectra of TbFe$_3$(BO$_3$)$_4$ displaying some more lines in low-temperature structural phase were interpreted on the basis of lowering of the symmetry at phase transition and additional Davidov splitting.

An anomalous temperature behavior of some vibrational modes was founded in magnetic phase. These phonon lines undergo a shift when an external magnetic field H || C$_3$ is applied.

A broad structured band around 70 cm^{-1} was observed at low temperatures and was attributed to two-magnon Raman scattering. The band displays no changes of shape, shifts or splitting in applied magnetic field. The energy of magnons on the Brillouin zone boundary was estimated.

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COMPARISON OF THE LUMINESCENT PROPERTIES OF EUROPIUM COORDINATION COMPOUNDS WITH DIFFERENT CARBACYLPHOSPHORTRIAMIDE LIGANDS

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In the past decade, in the context of the increasing use of luminescence spectroscopy for facing complex analytical problems in fields of large social and economical impact such as environmental sciences, medical diagnostics, and cell biology, lanthanide complexes have been the focus of much attention for their possible application as labels and sensors. Eu^{3+} ions, which possess luminescence lifetimes in the microsecond–millisecond range, offer the opportunity to efficiently exclude autofluorescence and light scattering, the most relevant interferences, particularly when biological material is involved.

The aim of this work is to study the luminescent properties of europium coordination compounds with carbacylphosphortriamides – geteroanalogues of β-diketones (Fig.).

R = N (ring) **(HL¹)**	
2,2,2–trichloro-N-(dipiperidin-1-yl-phosphoryl)acetamide	
R = N (ring with O) **(HL²)**	
2,2,2–trichloro-N-(dimorpholin-1-yl-phosphoryl)acetamide	
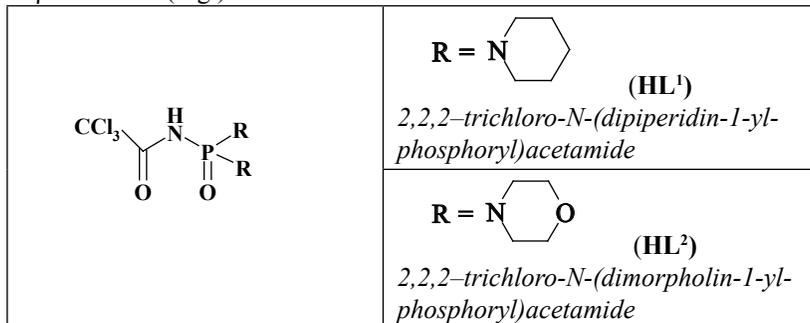
We used $Eu(NO_3)_2(L^1)(HL^1)_2$ and $Eu(NO_3)_2(L^2)(HL^2)_2$ crystal compounds that differ in the nature of the coordinated phosphortriamide ligands. Their luminescence spectra at 293 and 8 K have been reported and analyzed. In order to find out the ways of energy transfer to the luminescence center, the lasers with 337.1, 473 and 532 nm wavelengths were used. Luminescence of the HL¹ and HL² had also been excited in the maxima of their absorption bands lying in the UV- range of the spectra.

NONLINEAR LIGHT ABSORPTION BY IODINE IN 3D PHOTONIC CRYSTAL

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The confinement and guiding light in sub-wavelengths sized hollow core waveguides based on photonic crystal structure are very attractive tools for enhancement of light interaction with gas and vapour phase media with possible application to the miniaturization and simplification of existing measurement apparatuses. Nonlinear photon crystal based optical devices are particularly attractive because the light localization in photon crystal eliminates the tradeoff between small beam areas and finite focal depth. There are a number of potential applications of such systems in atomic and molecular spectroscopy, including gas phase sensing, precision spectroscopy, metrology etc.

Synthetic opals (opal lattices) constitute an important example of globular photonic crystals—systems consisting of spherical particles (globules) close packed in the form of a cubic lattice with a period a comparable to visible wavelengths. The periodic structure of photonic crystals leads to the formation of allowed and forbidden bands for photons (photonic bands). This feature of photonic crystals has been used to create advanced optical devices: high- Q resonators, spectral filters, and others [1].

The coherent Doppler narrowing of absorption line of cesium atom in a thin vapor cell and observation of the Dicke regime in the optical domain was demonstrated [2]. The similar effects could be observed in opal filled by absorbing gas.

The experimental equipment is based on the single frequency diode laser sub Doppler spectrometer [3]. The opal samples were placed in sealed cell, evacuated and filled by molecular iodine by vacuum sublimation techniques. The nonlinear absorption spectra were studied and results are discussed.

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4
LIQUID CRYSTALS

A DESIGN STRATEGY OF NEW MATERIALS WITH ACTIVE C=C BONDS FOR LC PHOTOALIGNMENT

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New polymer materials were designed for LC orientation under the illumination of linearly polarized UV light [9]. The main photochemical reaction which leads to the photoinduced optical anisotropy of their films is Fries rearrangement [2-7]. Materials proposed are bearing arylester photoactive fragments capable to Fries rearrangement and terminal tetrahydrophthalic/ maleimide/ methacrylamide groups capable of crosslinking due to photoaddition/ photopolymeryzation that in a case of polarized light illumination results in highly efficient LC alignment. To verify realization of each of these possible reactions IR spectra before and after UV irradiation has been analyzed [8]

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HELICAL TWISTING IN CHOLESTERIC SYSTEMS CONTAINING PHOTOSENSITIVE AZOXY NEMATICS: EFFECTS OF UV RADIATION

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For cholesteric liquid crystalline systems containing photosensitive nematic ZhK-440 and a mixture of cholesterol derivatives, changes in helical twisting induced by UV irradiation were studied. The UV-induced shift of the selective reflection maximum λ_{max} was shown to depend upon concentration of the nematic component. At low concentration of ZhK-440 λ_{max} increases, which correlates with corresponding temperature-induced changes. At higher concentrations of azoxy nematic, λ_{max} decreased regardless of the temperature behavior of the system. To explain the experimental data, a theoretical description is proposed on the basis of development of molecular models of helical twisting. Good agreement was obtained between calculated and measured values of UV-induced shift $\Delta\lambda_{max}$ as function of the azoxy nematic concentration, with two extrema and an inversion point. The extra twisting emerging in the system due to formation of non-mesogenic and non-chiral *cis*-isomers can be presumably assigned to ordered orientation of short molecular axes of *cis*-molecules, with resulting contribution to helical twisting determined by the sense of the helix that had been already formed in the cholesteric system.

In another set of experiments, cholesteric systems containing photosensitive nematic ZhK-440 and photosensitive optically active dopants were studied, and peculiar features of UV-induced variation of helical twisting in such systems are noted.

THE SPATIAL-PERIODIC THRESHOLD STRUCTURE OF DIRECTOR IN A NEMATIC CELL WITH PERIODIC ANCHORING ENERGY

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The threshold reorientation of director under the influence of static external electric field in a planar nematic cell with a periodic surface anchoring energy has been investigated theoretically. The value of transition's threshold and spatial distribution of director above the threshold have been found as functions of the period and anchoring energy value. It has been shown that the threshold of the transition depends non-monotonically on the number of anchoring energy periods s that could be located along the cell length. The distribution of director above transition›s threshold in the case of integer s traces the periodic changes of anchoring energy. The amplitude of per i - odic director›s deviations grows while the ratio of the cell thickness to the anchoring energy period decreases.

MAGNETIC HIGH-SENSITIVE DISPERSION OF MAGNETIC NANORODS IN NEMATIC LIQUID CRYSTAL

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Brochard and de Gennes in the 70th suggested that doping of thermotropicnematic liquid crystal (LC) with ferromagnetic particles of the micronsize could increase the magnetic sensitivity of the nematics on several orders [1]. Later [2] confirmed this suggestion, strong aggregation of ferro-particles in magnetic field prevented wide application of such ferronematics.

We report on studies of stability of the suspensions of ferromagnetic nanorods covered with different surfactants in a LC 5CB. To enhance the stability of dispersion the new surfactants were specially designed and synthesized. The surfactants consistedofa LC like molecule chain and phosphonic terminal group that provided a strong anchoring between surfactant and surface of the nanorods.
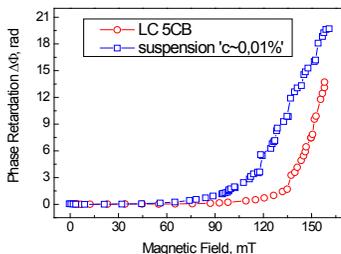
Dependence of the magnetically-induced phase retardation in the cells at the magnetic field.

Method of the particles preparation was described in [3, 4]. The resulting suspensions had different stability depending on the chemical structure of the surfactants. Neverthelessthe best suspensions revealed a good stability during at several months. The suspensionc=0,1% wt., was filled to the cell with a planar boundary conditions and put between cross polarizers in the magnetic field. We measured of the phase retardation in the cell in the magnetic field.

We found that the suspension was well responsive to magnetic fields. Doping with the particles decreased the Frederics threshold in the suspension on the 30-35% in compare the pure LC.

Taking into account the extreme sensitivity to magnetic field become the topical task of the physics and applications of ferronematics.

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STRONG CUBIC OPTICAL NONLINEARITY OF NEMATIC LIQUID CRYSTAL DOPED WITH GOLD NANOPARTICLES

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This paper reports on the observations of extremely strong and fast cubic optical nonlinearity in nematic liquid crystal (LC) doped with gold nanoparticles in the vicinity of a plasmon resonance band of the particles.

The nonlinearity was observed by recording dynamic phase sinusoidal holograms with a continuous operating laser. It is caused by changes of the refractive index of a LC due to efficient light-induced heating of the nanoparticles at plasmon resonance excitation and following thermal transport of heat to LC matrix.

Strong nonlinearity parameter ($n_2 \sim 10^{-2}$ cm^2/kW), fast characteristic times and excellent photo- and thermo-stability of the system exhibit several intriguing advantages for optical processing applications.

SIMULATING CHARGE TRANSPORT IN DISCOTIC LIQUID CRYSTALS

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The role of material morphology on charge carrier mobility in partially disordered organic semiconductors is discussed for several classes of materials: derivatives of hexabenzocoronenes [1], perylenediimides [2], triangularly shaped polyaromatic hydrocarbons [3]. Simulations are performed using a package developed by Imperial College, London and Max Planck Institute for Polymer Research, Mainz (www.votca.org,[4]). This package combines several techniques into one scheme: quantum chemical methods for the calculation of molecular electronic structures and reorganization energies, molecular dynamics and systematic coarse-graining approaches for simulation of self-assembly and relative positions and orientations of molecules on large scales; kinetic Monte Carlo and master equation for studies of charge transport.

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DIRECTOR FIELD IN A NEMATIC CELL WITH INHOMOGENEOUS ANCHORING

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Inhomogeneous alignment of liquid crystals (LCs) at boundary surfaces is important for both fundamental science and various technological applications. The competition between LC elastic energy and surface anchoring results in a rich variety of the director fields. Recently significant efforts have been directed towards designing patterned LC alignment with micro- and nano-patterns. These patterns can be achieved by various techniques such as nano-rubbing, nano-imprinting lithography, optical and chemical patterning, mixing polymers favoring planar and homeotropic alignment. Due to the small size of the pattern and relatively weak anchoring, elasticity can deviate the director at the inhomogeneous substrate from the easy axis. The similar effect may also be observed at the untreated substrates with 'random' alignment.

In this paper we present a theoretical description of the equilibrium director field in a nematic cell with inhomogeneous anchoring. We demonstrate that the elastic energy of the cell can be described by the director field at the inhomogeneous substrate, leading to a representation as a set of surface micro-domains with the effective interaction potential. We use this representation to perform numerical simulations and investigate dependence of director field on elastic constants, surface anchoring and cell thickness.

ELECTROOPTICAL AND NONLINEAR-OPTICAL PROPERTIES OF LYOTROPIC LIQUID CRYSTALS DOPED WITH ELECTROCHROMIC VIOLOGENS

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This work presents the results of experimental studies of structural, electrooptical and nonlinear-optical properties of lyotropic ionic liquid crystals (LILC) with soluted electrochromic admixtures of viologens.

It was obtained that LILC of potassium caprylate doped with viologen admixtures form double-layer smectic A phase which is characterized by electrostatic interlayer of metal cations, water, and negatively charged oxygen atoms between alkyl chains. It was found, that viologen molecules (2-4 % by weight) are harmonically built into liquid crystal matrix without breaking its order.

It was shown that LILC-viologen composites obtain electrochromic properties inherent to viologens, which produce coloured radical cations and dimers while reducing. The presence of radical cations and dimers is fixed by optical absorption spectra. It was established that under the action of an electric field samples of LILC-viologen form bi-layer structure consisting of a liquid crystal layer and an absorptive layer of viologen redox products (radical cations and dimers). Due to liquid crystal medium a deposited viologen layer is also characterized by ordering which was proved by the presence of dichroism in coloured samples.

A dynamic grating recording was realized and studied in bi-layer LILC-viologen cells. It was determined that recording takes place in the coloured layer of viologen redox products. The possible mechanism of grating recording in LILC-viologen cells was proposed.

PHOTOALIGNING OF LIQUID CRYSTALS ON INORGANIC SURFACE OF CHALCOGENIDE GLASSY FILMS

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The photoalignment of a LC on chalcogenide surface was firstly reported in [1]. Here we demonstrate photoalignment of different LCs by chalcogenide glassy surfaces and show a crucial role of the pair "LC – chalcogenide" for producing a light-induced anchoring. Our studies were focused on photoalignment of nematic LCs 5CB, E7 and E44 on a chalcogenide surface As_2S_3 at the in-situ irradiation with polarized light (l=436 nm). The experiments were carried out in the cells made of the command chalcogenide surface, the reference rubbed polyimide surface and LC in between. The initial planar unidirectional alignment on the chalcogenide surface was defined by the rubbed reference surface and by cooling of the cell from temperature T > T_c to the room temperature in a magnetic field parallel to the rubbing direction.

We found the evident dependence of the light-induced anchoring on the pair "LC- As_2S_3". The most efficient and stable anchoring was observed for the pair "5CB - As_2S_3". The pair "E7 - As_2S_3" revealed weaker anchoring that decreased with time. We did not find notable anchoring for the pair "E44 - As_2S_3". The director orientation induced by the first exposure could be reoriented by the second exposure with the different direction of light polarization. The observed results are explained in the frame of the model of light-induced adsorption/desorption of LC molecules with chalcogenide glass's absorption sensitivity to the light polarization.

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DIELECTRIC SPECTROSCOPY OF CHEMICALLY MODIFIED MOLECULES OF FULLERENE C_{60} IN NEMATIC LIQUID CRYSTAL

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We have obtained solutions C60 with attached molecules of diamine (C60D) in nematic liquid crystal 6CHBT. The concentration *c* of C60D in LC was changed within the range of 0 to 3 wt.%. We have studied samples of the sandwich structure of the thickness 25 μm with planar and homeotropic orientations of molecules. The film structure was investigated by using a polarizing microscope, and dielectric properties were studied within the range frequency 10^{-1}-10^{6} Hz and at the temperature 293 K by using an oscilloscope method [1].

For the frequencies less than 100 Hz, the dispersion of the components of complex dielectric permittivity was observed. It was shown that this relation can be described by the Debye equation. The value of relaxation time was determined. It was shown that the temperature dependence of relaxation time correlates with the temperature dependence of specific resistance.

As it follows from the analysis of dielectric spectra, for homeotropic orientation of molecules, the time relaxation τ caused by dipole polarization of molecules increases with the growth of the C60D concentration. For planar orientation, the value τ does not depend on the C60D concentration. It was shown that the parameters, which cover the temperature and concentration dependences of AC conductivity, also depend on an orientation of LC molecules. Analyzed were the reasons that explain these effects, and offered was the mechanism that interprets influence of structural features of C60D clusters on dielectric properties of the mixture LC- C60D.

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NONLINEAR OPTICAL RESPONSE OF SMECTIC GLASSES BASED ON COBALT ALKANOATES

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Metal alkanoates can form almost all states of condensed matter: solid crystalline state, liquid state, liquid crystalline state, isotropic and anisotropic glasses, and low-dimensional systems. Recently such a variety of metal alkanoates and their phase states was used in order to fabricate optical and nonlinear optical materials, for instance, double-layer cells "photosensitive film – ionic lyotropic liquid crystal", ionic lyotropic liquid crystals doped with electrochromic impurities [1], mesomorphic glasses with dissolved dye molecules [2].

In present work we studied nonlinear-optical properties of the mesomorphic glasses based on cobalt-alkanoates: i) homologous series of pure cobalt alkanoates; ii) binary and ternary systems based on cobalt\potassium\lithium octanoates. Nonlinear-optical response of anisotropic smectic glasses was studied using method of the dynamic holography. Laser induced dynamic gratings under the action of the nanosecond laser pulses were observed and analyzed for such materials. It was found that cubic optical nonlinearity of all studied anisotropic glasses is of electronic origin at nanosecond diapason and caused by nonlinear polarization of the cobalt-alkanoates complexes. Fundamental optical (refractive index n and absorption coefficient α) and nonlinear-optical (nonlinear susceptibilities $\chi^{(3)}$ and polarizabilities γ_{NL}) parameters of the mesomorphic glasses based on cobalt-alkanoates can be tuned via varying length of alkanoate anion chain (interlayer smectic distance) and by varying binary and ternary metal alkanoate systems.

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SUSPENSIONS OF FERROELECTRIC NANOPARTICLES IN LOW BIREFRINGENCE LIQUID CRYSTALS

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Colloidal dispersions of nanoparticles in liquid crystals are of great interest as they have advantage of combining the orientational order of liquid crystals and physical properties of nanoparticles. Such systems have a potential for the electro-optic displays because of their effective sensitivity to external fields [1]. Ferroelectric nanoparticles that are dispersed in a nematic liquid crystal macroscopically appear identical to a pure liquid crystal. However these colloids show interesting physical properties since strong electric field from the particles enhances the orientation ordering of liquid crystal molecules [2-3]. Recently it has been reported that the suspensions of ferroelectric nanoparticles in liquid crystals at low concentrations (~0.1%) increase the nematic-isotropic phase transition, optical anisotropy and dielectric anisotropy but decrease the threshold voltage [4].These changes in the physical parameters are due to the increased orientational order of liquid crystal molecules induced by ferroelectric nanoparticles. In this study we report the recent investigations of optical parameters of the ferroelectric nanoparticles in low birefringence liquid crystals and discuss order parameters of these colloids.

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MOLECULE LENGTH INFLUENCE ON THE STRUCTURAL PROPERTIES OF NORMAL ALKANE ELC LAYERS

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Structural characteristics of epitropic liquid crystalline (ELC) [1] layers of saturated hydrocarbons, which form the base of lubricating oils, determine anti-wear properties of the latest [1]. As it was defined by the hydrodynamic modeling approach [2] on the basis of rheological research, the thickness of normal alkanes ELC layers, in particular, which formation is related to the fluctuation forces generated by metal surfaces, may reach several microns ($\sim 1 \div 5$ µm). Although the influence of molecule chain length on the n-alkane homologues ELC layer structural characteristics, such as layer thickness and degree of ordering, is under consideration.

Estimation of structural parameters of ELC layers of $C_{13}H_{28}$ and $C_{17}H_{36}$ was performed using the variable thickness slot light guide method [1]. Within the framework of such approach, the dependence of phase shift δ between the elliptically polarized light ($\lambda_{Na} \sim 589$ nm) components on the thickness D ($\delta = f(1/D)$) of interlayer, bounded with metal substrates, is established and structural parameters are defined:

$$\delta = \frac{2\pi}{\lambda} L (2d_s \Delta n) \frac{1}{D}$$

where d_s is the ELC layer thickness; Δn is the value of optical anisotropy, which determines the degree of molecule ordering; L is the light guide length.

It was determined that ELC layer thickness of $C_{17}H_{36}$ ($d_s \sim 4$ µm) and value of Δn ($\Delta n \sim 1,8 \cdot 10^{-5}$) at the metal substrate are higher compared to $C_{13}H_{28}$ ($d_s \sim 2$ µm, $\Delta n \sim 1,35 \cdot 10^{-5}$). This may be explained as increase of layer degree of ordering within the molecule chain length.

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PHOTOCONDUCTIVITY OF 4-PENTYL-4'-CYANOBIPHENYL IN DC FIELD

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Nematic liquid crystal (LC) 4-pentyl-4cyanobiphenyl 5CB has recently attracted significant attention as photorefractive medium. There two types of photorefractive effects in this material which are observed at dc-field applied to the LC cell. The first one is related to bulk-mediated photorefraction [1-2]. In this case incident light intensity grating generates photo-charges in LC bulk, which migrate and diffuse within the LC material and set up spatially distributed charge field. The second one is related to surface-mediated photorefraction [3-5]. In this case the space-charge grating is formed in the "aligning layer-LC" interface. The spatial modulation of the charges in the interface results the corresponding modulation of the electric field which extends in the LC bulk and reorient the director. The characteristics of the surface-mediated photorefraction gratings strongly depend on the characteristics of LC electrical double layer nearby the aligning surfaces and related to photoconductivity in the LC cells. We report on studies of formation of the charges double layer and photocurrent characteristics in a cell with two ITO-boundary surfaces and LC 5CB in between. It was found that optimal characteristics of the photorefraction grating recording which realized at the applied dc-field correspond to the formation of the stationary charges double layer at the ITO surface. The irradiation of the interface results in a shrinking of the
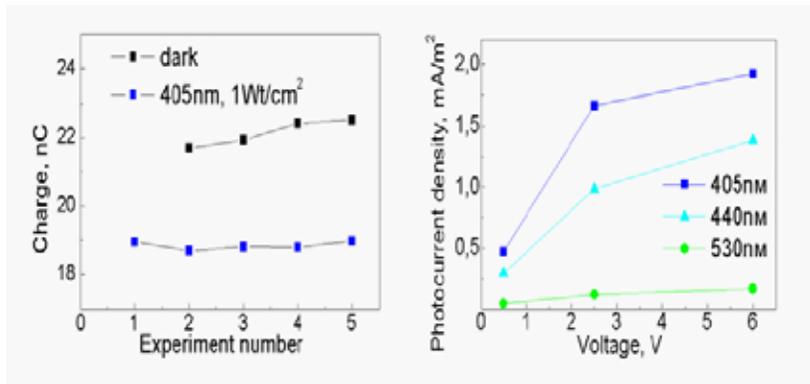
double layer (Figure, left), producing of a photoconductivity which changes the value of the initial steady current in the cell (Figure, right).

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REORIENTATION OF LYOTROPIC FERRONEMATIC IN A MAGNETIC FIELD

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The idea of imparting ferromagnetic properties to nematics by doping liquid crystals with ferromagnetic nanoparticles, proposed by De Gennes and Brochard many years ago [1], opened the field of hybrid liquid-crystal composites. Here, we report on basic properties of new liquid-crystal nanomaterials based on dispersions of ferromagnetic nanoparticles in mineral liotropic liquid crystal.

We used a colloidal aqueous suspension of V_2O_5 ribbons (several 100 nm long, about 25 nm wide, and 1 nm thick) doped with ferromagnetic Fe_3O_4 spherical particles of 10 nm diameter. Undoped colloidal suspensions displayed a nematic phase for V_2O_5 volume fractions in the range of $0.7 - 1.1$ %. Doping of the V_2O_5 colloid with Fe_3O_4 nanoparticles resulted in a shift of the nematic range to smaller volume fractions. The nematic colloids were studied in 50 mµ thick cells made from two glass substrates, covered with either ITO layer or with a surfactant , $C_nH_{2n+1}O(CH_2-CH_2O)_m$ (*n* 12-14; *m* = 10) layer. The planar alignment of the colloids was achieved by flow during cell filling and was stable for weeks. No aggregation of V_2O_5 ribbons and ferromagnetic nanoparticles was observed either by polarizing microscopy or by small-angle X-ray scattering.

We found that the colloidal hybrid (V_2O_5/Fe_3O_4) nematic dispersion is very sensitive to a magnetic field. The field, H , was applied perpendicularly to the cell substrates and we measured the dependence of the optical phase retardation in the cells on field intensity. The phase retardation in the cells with pure V_2O_5 nematic colloid did not show any change up to the highest available field, $H = 2.5$ kG (the reorientation threshold for this colloid was reported to be about 10 kG [2]). In contrast, phase retardation changes, without any threshold, were observed with the (V_2O_5/Fe_3O_4) doped colloid; direc-

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tor reorientation was readily observed at $H \geq 50$ G. The characteristic times of director reorientation were around several minutes and decreased with the increasing field intensity.   Switching off the field resulted in slow (~30 min) relaxation of the director back to the initial state. This recovery of the initial alignment suggests the existence of an anchoring energy of the suspension, which is probably due to anisotropic interaction of ribbons with the aligning surfaces.

To set the origin of the effect we studied the magnetically-induced bire-fringence of the dispersion of the nanoparticles Fe_3O_4 in water and of (V_2O_5/Fe_3O_4) isotropic dispersion in water. It was shown that at the same concentra-tion of Fe_3O_4 nanoparticles the field-induced birefringence in the isotropic V_2O_5/Fe_3O_4 dispersion was in two orders larger than in Fe_3O_4 dispersion. In the limit of one order smaller volume concentration of Fe_3O_4 nanoparticles than volume concentration of V_2O_5 this birefringence is proportion to the concentration of Fe_3O_4 . These facts together with other results have allowed us to suggest a mechanism of the extra-high sensitivity of the V_2O_5/Fe_3O_4 dispersion based on formation of chain-like structures of Fe_3O_4 particles in the dispersion, oriented along H-field. An electric interaction between these anisometric chain structures and V_2O ribbons induces in a strong torque that results in the reorientation of the V_2O_5/Fe_3O_4 dispersion.

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FERROELECTRIC-LIKE CURRENT –VOLTAGE AND CHARGE VOLTAGE LOOPS OF COLLOIDS OF SrTiO$_3$ NANOPARTICLES IN NEMATIC LIQUID CRYSTALS

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Colloids of nano-particles (NP) of different nature in liquid crystal (LC) host possess intrigue properties, especially the colloids of ferroelectric (FE) nano-particles (FENP) in nematic LCs. Advanced properties were attributed to spontaneous polarization P$_s$ of the FENP. Earlier we observed the polarization reversal-like behaviour in FENP-LC colloids with Sn$_2$P$_2$S$_6$ and BaTiO$_3$ (BTO) NP.

To clarify a crucial role of P$_s$ in the observed ferroelectric-like behaviour of FENP-LC colloids we performed the same characterization for NP-LC colloids with NP of quantum paraelectric SrTiO$_3$ (STO), which belongs to perovskite group as ferroelectric BaTiO$_3$, but does not possess P$_s$ even under deep cooling.

The (0,1-1) vol % NP-LC colloids of STO (50-80 nm) nanopowder in LC pentylcyanobiphenil (5CB) and NP-LC-cells were prepared the same as FENP-LC-cells, namely NP were covered with an oleic acid (OA) surfactant and the layer of polyvinyl-cinammate (PVC) was used for LC planar alignment.

The studies of dynamic charge-voltage (Q-V), current-voltage (I-V-) and capacitance-voltage (C-V-) loops were performed. Drive a.c. voltage of 0 - 20V of amplitude in the frequency range 0,1 Hz - 1 kHz was applied to the circuits of series connection of tested sample with reference capacitor or resistor.

The shapes of experimental I-V-, Q-V- and C-V- loops for BTO FENP-LC and STO NP-LC colloids are qualitatively similar, in particular the I-V-loops contain the characteristic peaks that indicate coercive-like phenomena. Under the same conditions the characteristic current peaks are not observed in the LC-cells with pure 5CB. Only in general the shape of I-V- and Q-V-loops of BTO FENP-LC and STO NP-LC colloids is similar to that of non-saturated I-V- and Q-V-loops for BTO single crystal plates. The peculiarities of I-V-, Q-V-and C-V- loops and frequency behavior of I-V- and Q-V-loops similar for both types of colloids are different from those of FE plates.

The behaviour of BTO FENP-LC and STO NP-LC colloids is discussed related to LC dimer – LC monomer local orientation transformation, surface anchoring and adsorption influence on local director configuration, different boundary conditions at (NP)OA – LC and LC – PVC surfaces, and space charge and field effects in (NP)OA – LC and (NP)OA – LC – PVC–ITO-electrode inter-spaces.

POLARIZATION DIFFRACTION GRATINGS IN LIQUID CRYSTALS CELLS WITH CHALCOGENIDE GLASSY COMMAND SURFACE

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We report on recording of permanent electrically-controlled polarization gratings by means of polarization sensitive light-induced anchoring of liquid crystals (LCs) on photosensitive chalcogenide glassy surface. The gratings were recorded in the combined LC cells with cell gap around 30 mm. They consisted of command chalcogenide $As_{20}Se_{80}$ surface, reference surface and the LC 5CB or E7 in between. The rubbed polyimide layer served as the reference surface. It provided strong planar alignment of the LC. The command chalcogenide surface was also rubbed. The directions of rubbing on the command and reference surfaces were parallel. The cells were filled with the LCs in nematic phase by capillary effect and a uniform planar alignment of LCs was formed. To record the gratings, two laser beams with $l = 532$ nm and opposite circular polarizations were intersected in the plane of the cells. It resulted in a spatial modulation of the linear polarization, $\vec{E}(x)$, with a period determined by the converging angle of the recording beams. Due to the effect of light-induced anchoring, the spatial modulation $\vec{E}(x)$ resulted in modulation of the easy orientation axis of the LC on the chalcogenide surface, $\vec{e}(x)$. The spatial distribution $\vec{e}(x)$ led to the corresponding modulation of the optical axis in the LC bulk and resulted in recording of the grating. The grating was tested by observation of the probe beam diffraction. Application of the electric field resulted in the reorientation of the LC and a change of the phase retardation amplitude modulation in the cell. It allowed us to effectively control the diffraction of light and to optimize the diffraction efficiency of the grating. The maximum diffraction efficiency h » 33% was achieved.

High sensitivity and thermal stability of the grating in LC cells with chalcogenide layers together with effective electrically driven control of the gratings characteristics makes them very attractive for potential optical and photonics applications.

INFLUENCE THE QUALITY OF THE PLANAR TEXTURE OF A CHOLESTERIC LIQUID CRYSTAL ON THE LASING SPECTRA

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Dye-doped chiral liquid crystals (CLC) with a natural periodic structure suitable for lasing. On the basis of such materials microlasers with distributed feedback have been realized (DFB) [1]. Low lasing threshold and the arbitrary size of the active medium of such lasers are responsible for the prospects of their use in creating new systems of information displays.

The goal of our work was to study the effect of the optical quality of the planar texture of the steroidal CLC on the spectral characteristics of lasing.

Used three methods to create a planar texture of the steroidal CLC; orientation by rubbing in the one direction of substrates with polyimide varnish (PAC) deposited on transparent electrodes of SnO_2; only substrates with a layer of PAC and substrates with a layer of polyvinyl alcohol (PVA). The lasing spectra in a CLC at different methods their orientation show strongly correlation with the quality of the texture. For the best quality texture with a narrow band of selective reflection (SR) (the orientation of the CLC layer by $PAA + SnO_2$) in the lasing spectrum recorded three lines, which correspond to longitudinal modes with a low lasing thresholds. Expansion of CO bands in the texture produced by the two other technologies, accompanied by a broadening of the mode structure in the lasing spectrum and increasing her threshold.

An interesting result was obtained with additional orientation viscous steroidal CLC rotation for 90^0 either of the orienting substrates. In such a texture recorded the most narrow SR band, in the lasing spectrum was observed only one central mode. The lasing thresholds for the two side modes is not achieved even with a substantial (50 times) increase in the pump. A possible explanation of this phenomenon - the formation of local defect mode due to the phase jump at turn orienting the substrate [2]. Obtained results allow us to define the limits of applicability of existing models of the lasing to specific types of CLC.

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PHOTOINDUCED OPTICAL ANISOTROPY INVESTIGATION IN POLYMETHACRYLATES WITH SIDE-CHAIN AZOBENZENE MOIETIES

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In the past few years, azo-dye-containing polymers have been the subject of intensive research because of their potential uses in photonics, optoelectronics, and optical signal processing. One of the main interests of these polymers is photoinduced optical anisotropy, which is appeared when they are irradiated with the linearly polarized light. This phenomenon comes from the reorientation of the azobenzene groups through trans-cis-trans isomerization cycles, which leads to an excess of photochromic entities oriented perpendicularly to the laser polarization direction.

$$R = NO_2, COOC_4H_9, OCH_3, OC_5H_{11}$$
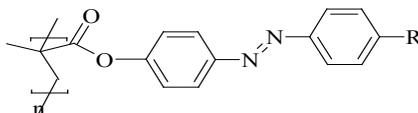
In this work we study the kinetics of the photoinduced orientational ordering of two type of methacrylic polymers containing different azobenzene groups with both electron-donor and electron-acceptor substituents under irradiating them at two different wavelengths. For the experimental study of the orientational distribution in polymer films we use the methods of null ellipsometry and polarization spectroscopy [1]. It was found that azo fragments were oriented by photoorientation or photoselection mechanisms depending on the excitation wavelength as well as the end substituents in azo fragments. In the case of acceptor substituents (NO_2, $COOC_4H_9$), azo fragments adopt a uniaxial orientation and a uniform distribution in the plane perpendicular to the direction of excitation-light polarization. In the case of donor substituents (OC_5H_{11}, OCH_3) the distribution of azo fragments in the saturation state is isotropic at the excitation of the wavelength corresponding trans-isomers. Irradiation them of the wavelength corresponding cis-isomers leads to orientation, which is the same as in the case of acceptor substituents.

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EFFECT OF MODIFICATION ON THE ADSORPTION PROPERTIES OF SMALL AMOUNT OF SINGLE-WALL NANOTUBES IN THE NEMATIC MATRIX

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Prepared and studied were stable for several months mixtures of nematic liquid crystal 6CNBT with single-wall carbon nanotubes (CNTs), which were unmodified and modified with COOH groups. The diameter of nanotubes was 10 nm, the length was 1000 nm, and the concentration – 2.10 wt.%. The samples with planar orientation of LC molecules were prepared by deposition of orienting coatings. Observations with the polarizing microscope showed that a low concentration of nanotubes does not effect on the orientation of liquid crystal molecules.

Using the oscilloscope method within the frequency range 10^{-1}-10^6 Hz and at the temperature 297 K, dielectric properties of the obtained mixtures were studied. It was shown that even a small amount of nanoparticles leads to changes of the sample properties.

It was shown that, unlike the LC mixtures with high concentration of nanotubes , the presence of small amount of nanoparticles leads to a decrease in the conductivity of the mixture LC-NTs. The maximum decrease in the conductivity was obtained for LC mixtures with the modified NTs (more than three times). Non-modified NTs reduce the conductivity of the mixture by two times less than the modified ones. It was suggested that the main reason for the reduction of conductivity is adsorption of ions, which are located in LC and take part in charge transfer on the surface of nanotubes. Modification of NT by the COOH group leads to a significant increase in adsorption properties of the NTs. Estimations were made as regard to improvement of the adsorption properties of NTs by using other groups of molecules apart from the COOH ones.

EFFECTS OF LIQUID CRYSTALLINE PHASE STATE UPON LUMINESCENT PROPERTIES OF 2-BROMOBENZOPHENONE

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Luminescence spectra of liquid crystalline solutions of 2-bromobenzophenone (2BrBP) were studied in comparison with similar spectra of 2BrBP measured in standard organic solvents and in the crystalline form. The luminescence behavior was found to be markedly different at different excitation wavelengths. Under 280 nm excitation, the luminescence spectrum was generally similar to that obtained in a standard (isotropic) solvent with a characteristic band peaked at ~322 nm, though a strong long-wave tail could be noted. Under 240 nm excitation, the 322 nm band completely disappeared, and a broad luminescence peak emerged at ~420 nm, rather close to the 437 nm and 467 nm peaks noted for the crystalline samples for both excitation lengths. Moreover, several additional peaks in the ~350-425 nm range appeared in the standard solution under 240 nm excitation, alongside with the 322 nm band.

The observed unusual behavior can be considered as an even more clear example of the effects of liquid crystalline phase state upon luminescent properties in the case when the luminophores show molecular polymorphism [1]. Apparently, in this case molecular luminescent properties are affected not only by conformational changes induced by orientationally ordered medium, but also by conformational changes under excitation, with a complex interplay of both factors.

Another interesting property of 2BrBP is its very high (up to 20%) solubility in liquid crystal solvents. Its effects upon helical twisting, studied under the same conditions as previously reported for other luminophores [2], at high concentrations become notably non-linear, with induction of texture changes within the cholesteric mesophase.

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ORIENTATION PROPERTIES AND INTERACTION OF NEMATIC LIQUID CRYSTALS WITH NEW PHOTOSENSITIVE AZOMETHINE POLYMERS

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We report the development and characterization of new photosensitive polymers for orientation of nematic liquid crystals (NLCs). These materials based on azomethine polymers and have different arrangement of chromophores. We found that polymers demonstrated high photosensitivity and rather strong anchoring energy of liquid crystals. The reference cell technique [1] was used for estimation of the azimuthal anchoring energy. The poliazomethines that contained chromophores in the main chain were obtained through polycondensation of aromatic dialdehydes with some aromatic diamines. These polymers demonstrated the increase anchoring energy of liquid crystals during the observation period. The polymers that contained chromophores in the side chain were synthesized by the reaction of azomethine dyes with 2-methylacryloyl chloride followed by the polymerization in DMF at 80 °C in the presence of AIBN as a free-radical initiator. These polymers clearly demonstrated the decrease anchoring energy of liquid crystal during our experiments. The photoalignment mechanisms are discussed in terms of dispersion and dipole-dipole interactions between liquid crystal molecules and photosensitive polymer fragments.

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NEW METHACRYLIC AZOPOLYMERS AS MATERIALSFOR LIQUID CRYSTAL PHOTOALIGNMENT

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The phenomenon of photo-alignment and new photo-aligning materials were subjects of extensive researches, since the effect was firstly described as reversible cis-trans isomerization of the azobenzene units attached to the substrate or polymer matrix. Photo-alignment is a non-contact method, which enables to create a high quality orientation of the liquid crystal (LC) layer without mechanical damage of the substrate, electronic charge or dust contamination. After the appearance of the first photo-aligned films, such as dye-doped polymer layers [1] or polyvinyl cinnamates the development of new photo-aligning materials becomes a hot topic of research [2].

In this work, we concentrate on the methacrylic azopolymers of different structure with both electron-donor and electron-acceptor substituents.

These polymers were obtained by free-radical polymerisation of such methacrylic azobenzene-containing monomers as:
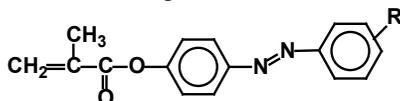
where R = CH_3, OCH_3, NO_2, Br

Copolymers were synthesized from azobenzene-containing monomers with methyl-, butyl- octyl-, decylmethacrylate as well as 2-hydroxyethyl-methacrylate in AIBN-catalyst presence.

We have investigated the photo-aligned azopolymer layers for liquid crystal alignment and studied its dependence on azobenzene chemical structure as well as main polymer chain.

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THE INFLUENCE OF LIGHT BEAM'S NARROWNESS ON THE HYSTERESIS OF FREEDERICKSZ TRANSITION IN A NEMATIC CELL

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The influence of incident light beam's narrowness and intensity distribution along beam's transverse dimension on the hysteresis of light induced Freedericksz transition in a homeotropic nematic liquid crystal cell has been considered. Cases of one- and two-dimensional confined beams have been investigated. In the case of one-dimensional confined beam several different distributions of the light intensity have been used for calculations. Threshold values of orientational instability and values of maximal director's jumps for increasing and decreasing of the incident light intensity have been found numerically as functions of beam's transverse size. Conditions for the maximal width of the hysteresis loop have been obtained. It has been demonstrated also that the range of admissible elastic Frank constants' ratios $(K_3 - K_1)/K_3$ and K_2/K_3 becomes wider with increasing of the transverse size of one-dimensional confined light beam.

THE INFLUENCE OF RIGIDITY OF CHIRAL STEROID CORE IN MOLECULAR STRUCTURE OF CHIRAL DOPANTS ON SHORT-PITCH TEMPERATURE DEPENDENCE

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Among experimental studies the certain interest is devoted to investigations of character of temperature dependence of helical pitch in visible range, l, for cholesteric liquid crystal (LC) systems induced by chiral dopants. There are some origins to be responsible for this characteristic.

Since $l = P \cdot n$, the temperature dependence of mean refractive index, n (T), yields some contribution, but in the majority of cases, n (T) dependence of different nematics is quite negligible. The change of elastic constants of selected nematic with temperature effects on character of l (T) and gives one more additional contribution. But we believe the most important factor determining the certain dP/dT (and correspondingly, dl/dT) is the possibility of conformational changes with temperature in molecular structure of a chiral dopant, if it takes place or, contrary, relative molecular rigidity of a chiral dopant. The latest aspects are widely discussed in literature. The helical pitch gradient with temperature is usually observed for flexible chiral compounds [for example, 1]. The effect of molecular rigidity, for example, in case of bridged biaryl and helicene derivatives is mentioned as a reason of little temperature dependence of helical pitch [2].

In this work we discuss some 5α-androstanone, androstenone and estrone derivatives possessing relative rigid molecular structure due to inflexible steroid core and its influence on the helical pitch temperature behavior in induced cholesteric LC systems.

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HYDROGEN BONDS AND MESOMORPHISM OF CHOLESTERYL FORMIATE

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1. Introduction. Cholesteryl formiat (ChF) is the first member of cholesteryl n-alkanoates homologous series. ChF has a monotrop cholesteric liquid crystal phase which appears under cooling of the isotropic ChF phase [1]. IR spectra have shown [2] that in ChF there are intermolecular hydrogen bonds. The purpose of the given work is to provide more detailed and correct, as compared with [2], study of hydrogen bonding in ChF and its influence on mesomorphism of ChF.

2. Methods. ChF in solid crystal, cholesteric liquid crystal, and isotropic liquid phases as well as in solution in the CCl_4 was investigated by IR spectroscopic method. Infrared absorption spectra in the 4000-400 sm^{-1} region were measured by spectrophotometer UR-20. Besides, ChF was studied by a method of semi empirical quantum-chemical calculations.

3. Results and discussion. Changes of IR spectra in the basic in the 1750-1700 sm^{-1} region of C=O stretching vibration at phase transitions show that in ChF there are intermolecular hydrogen bonds of type C=O…H-C. In solid crystalline phase all molecules are associated on dimers. In isotropic liquid phase almost all dimers are dissociated on monomers. In cholesteric liquid crystal phase the number of dimers and monomers is almost equal.

Semi empirical quantum-chemical calculations confirm these results.

4. Conclusions. Formation of intermolecular hydrogen bonds in solid crystal phase of ChF leads to increase of forces of intermolecular interactions, and, as consequence, to rise in temperature of melting of ChF. Transition from at solid crystal phase to isotropic liquid phase without formation liquid crystal phase at heating of crystal ChF can be explained by the fact that the temperature of melting of ChF lies above temperature of area of existence of the mesophase.

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5
NANOOBJECTS

STRUCTURAL AND PHOTOLUMINESCENCE PROPERTIES OF ZnO/SBA-16 NANOCOMPOSITES OBTAINED BY SUBLIMATION METHOD

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Nanoscale semiconductor materials are currently in a focus of considerable interest due to their great potential for the application as functional materials. Due to its wide band gap and high exciton binding energy the nanosized ZnO is one of the most promising materials for applications in UV light emitters, transparent conductive films, gas sensing, etc. Wide variety of ZnO nanoparticles has been synthesized. Among them the nanoparticles encapsulated in inert matrices are advantageous due to better stability of their surface conditions. Many porous materials have been used to prepare ZnO nanostructures: zeolites, porous silicon, porous alumina, porous carbons, and porous silicas. Among these nanoporous solids, the SBA-16 silica has attracted a lot of attention because of its three dimensional cage structure, high surface area, relatively high pore volume, large pore sizes, good thermal stability due to the thick wall, and economical synthesis with inexpensive silica sources.

This study is focused on the synthesis and characterization of nanocomposites constituted of ZnO nanoparticles dispersed in mesoporous silica matrix SBA-16. Mesoporous silica SBA-16 was prepared using the non-ionic triblock copolymers Pluronic F127 ($EO_{106}PO_{70}EO_{106}$) as template. Molar ratio of the components in the starting mixture of reactants was: 1 TEOS : 0,004 F-127 : 4,2 HCl: 119 H_2O. All the used chemicals were analytical-grade reagents. SBA-16 thus synthesized has a cubic arrangement of mesopores corresponding to the Im3m space group. Textual properties of SBA-16 are pore volume V= 0,52 cm^3/g, BET surface area S_{BET} = 589 m^2/g, cage size = 71 Å.

The nanoparticles are grown inside the matrix by the sublimation method. This novel route of synthesizing ZnO nanoparticles implies physical sorption of zinc acetilacetonate precursor into the matrix pores from the gaseous phase, hydrolysis of the precursor, and thermal decomposition of the product with the formation of ZnO nanoclusters directly inside the pores. The

procedure of SBA-16 loading with ZnO was carried out in a two-chamber evacuated vessel. The nanocomposite was characterized by X-ray diffraction (XRD), nitrogen adsorption-desorption isotherms, and photoluminescence spectroscopy methods.

Small-angle X-ray diffraction patterns for the pure SBA-16 porous silica and the nanocomposite material revealed one strong diffraction peak and two minor less-resolved higher angle peaks in the range of $2\theta = 0.8$–$1.8°$, assigned to (110), (200) and (211) planes. Observation of this diffraction peak points to the presence of periodically organized mesoporous structure with regular repetition of the pore diameter. The position of the reflection peak is the same both for pure SBA-16 and ZnO-containing composite, and the intensity of the peak does not change essentially after the introduction of ZnO into the porous matrix. This proves that the ZnO-containing matrix maintains the same order, i.e. maintains the same size of the unit cell upon ZnO loading and subsequent treatments.Thus, introduction of ZnO does not affect the mesoscopic order in the host.

The high-angle XRD patterns in nanocomposite ZnO/SBA-16 show no characteristic peaks of the wurtzite ZnO structure. The absense of diffraction maxima could be attributed to the formation of very small zinc oxide clusters in the pore system of mesoporous silica matrix SBA-16 by a sublimation method. This suggestion is further supported by the chemical analysis results.

Nitrogen adsorption–desorption isotherms of pure SBA-16 and ZnO/SBA-16 nanocomposites are all type IV classification, which is characteristic of adsorption of mesoporous materials. The decrease of BET surface area, average pore diameters and pore volumes with the loading of ZnO indicates that ZnO clusters should be confined in the pores of SBA-16.

The photoluminescent properties of the pure mesoporous silica SBA-16 and of the ZnO/SBA-16 nanocomposites were characterized by the photoluminescence measurements with the excitation wavelength of 337 nm at room temperature. The ZnO/SBA-16 nanocomposites yield a strong emission band at about 381,8 nm.

The photoluminescence results with the ones of X-rays diffraction and nitrogen adsorption-desorption methods demonstrate that the proposed sublimation method of synthesis of the ZnO/SBA-16 nanocomposites provides good luminescent material.

ENERGY MIGRATION IN PSEUDOISOCYANINE J-AGGREGATES

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Luminescent molecular aggregates (so-called J-aggregates) take a special position among organic materials, due to their very narrow absorption band, near resonant luminescence, giant oscillator strength, giant optical nonlinearities, high sensitivity of spectral properties to the microenvironment. These features are caused by delocalization of the excitation over a molecular chain and Frenkel excitons appearing. One of the fundamental question in J-aggregates photophysics is an exciton migration. There is a significant contradiction in the efficiency of exciton energy migration reported by different authors. According to some data the exciton migrates in J-aggregates over up to several hundred molecules, while in other data an exciton motion over 10^4 molecules at room temperatures is stated. Using exciton traps, recently, we have shown efficient exciton migration in J-aggregates of amphiphilic pseudoisocyanine (amphi-PIC) dye. But the most interesting is to estimate the exciton transport efficiency in pseudoisocyanine (PIC) dye, which is the most investigated J-aggregating dye.

To achieve this goal another cyanine anionic dye DiD-C3S has been used as an exciton trap. As PIC is cationic dye, the main attractive force for DiD-C3S incorporation into PIC J-aggregates was the Coulombic interaction. Despite it, sensitized luminescence of the trap incorporated into PIC J-aggregates in solution has been revealed to be quite low, pointing to weak interaction. An analysis of J-aggregates luminescence quenching by the DiD-C3S dye using Stern-Volmer equation has shown that 50% of PIC J-aggregates luminescence is quenched in ratio PIC/DiD-C3S = 12:1, that is much less compared to amphi-PIC J-aggregates (amphi-PIC/trap = 120:1) . Formation of surfactant shell around PIC J-aggregates, which improves it structure, leads to increasing the exciton migration efficiency.

Formation of the PIC J-aggregates in PVA polymer films using spin-coating method helps to concentrate traps and J-aggregates that result in stronger interaction and increasing DiD-C3S sensitized luminescence. Using Stern-Volmer equation it has been shown that 50% of PIC J-aggregates luminescence in films is quenched in ratio PIC/DiD-C3S = 28:1, i.e. exciton migration efficiency in J-aggregates dispersed in polymeric film is increased comparing to that in solution.

PHOTON-BOSON CONVERSION IN PHOTONIC CRYSTALS

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The results of experimental and theoretical investigations of "up" and "down" conversion of light emission effects in media and in photonic crystals are presented. Secondary emission properties of globular photonic crystals, constructed from SiO_2-globules (200-600 nm) and filled by different luminophors [1-2] are discussed.

Stimulated and spontaneous photon-boson conversion effects are analyzed. The conditions for observation of visible photon conversion into scalar or pseudoscalar quasiparticles in crystals, photonic structures and in physical vacuum are discussed [3-5].

The applications of photon-boson conversion for construction of selective and conversional mirrors in lasers are described. Solar light photovoltaic elements, supplied by photonic crystal converters, should provide increased efficiency.

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ENHANCEMENT OF THE IR-SIGNALS OF BIOORGANIC MOLECULES ADSORBED ON THE SURFACE OF CARBON NANOSTRUCTURES

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Unique properties of the plane and rolled graphene sheets (carbon nanotubes), fibers, exfoliated graphite, etc., are of fundamental and applied interest. Earlier we have studied thymine (Thy) and adenine (Ade) interaction with single walled carbon nanotubes (SWCNT) with IR-experiment and quantum-chemical calculations. We found numerous structural changes in Thy and Ade molecules under their adsorption on single walled carbon nanotubes. Recently we paid attention to an enhancement of IR signals for a number of bands of Thy and Ade adsorbed on the SWCNT surface. The enhancement factor of IR main bands of Thy and Ade adsorbed on the surface of SWCNT was equalled to 2-10. The most enhancement in IR spectra was obtained in the region of low-frequency vibrations of the molecules under study. The effect of the enhancement of IR bands was registered by us for other molecules – sodium dodecyl sulphate, caffeine, DNA adsorbed on the SWCNT. This effect is similar to well-known surface enhanced infrared absorption (SEIRA) of the molecules adsorbed on the nanostructured metal surface. By the way, the carbon nanotubes could have metallic nature also. The mechanism of enhancement of vibrations of the molecules adsorbed on the graphene surface is discussed.

FLUORESCENCE RESONANCE ENERGY TRANSFER AS A TOOL TO STUDY DYE–TO–DYE INTERACTION IN NANO-SCALE VOLUME

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Recently, significant advances have led to a large variety of labeling reagents based on nanomaterials, such as quantum dots, magnetic nanoparticles, lanthanide doped-compounds, fluorophore-tagged latex/silica nanoparticles, fluorophore–labeled polymeric nanospheres etc. 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. Fluorophores can be introduced in non-fluorescent nano-scale objects either by covalent-labeling (fluorescent labels) or by adsorption (fluorescent probes). Both methods are widely applicable.

In the present study, it has been shown that fluorescence resonance energy transfer (FRET) between several dyes encapsulated in nano-scale volume is as effective tool for fluorophore-tagging of nano-sacle particles and studding dye–to–dye interactions in nanoscale volume. Sodium dodecyl sulfate (SDS) micelles and phosphatidylcholine liposomal vesicles have been used as model systems of nanoparticles. It has been shown that to create FRET composition in nano-scale volume, tandem dyes mast meet not only primary FRET requirements, but should have similar molecular topology and electronic density distribution. Using carefully selected dye molecules with extra-high FRET efficiency, the tags emission spectrum can be turned so that only the longest-wavelength dye will exhibit significant fluorescence at a short-wavelength excitation. This feature will overcome the challenge of small Stokes shift of many organic dyes. In our case, the "Stokes shift" of about 8000 cm^{-1} has been achieved. On the other hand, using dyes with different FRET efficiency, barcode tags can be produced for multiplexed targeted FRET under single wavelength excitation.

NEW NONLINEAR OPTICAL MATERIALS FOR PHOTONICS.

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New nonlinear optical materials were obtained on the basis of ionic liquid crystals and anisotropic glasses of pure metal alkanoates as well as with doping by different electro-photosensitive organic or inorganic additives and /or contain nanocrystals CdS. The molecular formula of metal alkanoates is $(C_nH_{2n+1}COO^-)_kM^{+k}$, where Me^{+k} – uni-, bi-,or tervalent metal cation, $C_nH_{2n+1}COO^-$ - alkanoate-anion, k = 1-3. These materials were synthesized by Institute of General and Inorganic Chemistry NAS Ukraine. Metal alkanoate salts can form lyotropic and thermotropic ionic liquid crystals and as well as anisotropic glasses at room temperature. The techniques for fabrication of the following cells were developed: 1. Double-layer composites: nanosized photosensitive dye or electrochromic viologene film – lyotropic ionic liquid crystals; 2. Mesomorphic glasses doped with organic or inorganic dyes and anisotropic glasses of alkanoates Co as well as binary and ternary mixtures of alkanoate metals containing alkanoate Co; 3. Anisotropic glasses of Cd alkanoates comprising CdS quantum dots. New materials manifest fast nonlinear optical response accompanied with small thermal effects within the light absorption range.

For dynamic holographic recording of grating we proposed covering thin absorbing dye film with ionic smectic lyotropic liquid crystals. Binary systems water – potassium caproate (H_2O- $C_9H_{19}COOK$, weight ratio of 1:1) were used as ionic lyotropic liquid crystals to cover absorbing thin dye film. Cationic and anionic polymethine dyes were used to fabricate thin absorbing film. Such double-layer cells were used for dynamic holographic grating recording. Ionic lyotropic liquid crystals (potassium caprylate) initially were doped with electrochromic dopants – viologens. Such a mixture of ionic liquid crystals and viologens is transparent initially but drastically changes its color when a DC electric field is applied to the cell, demonstrating a typical electrochromic behavior. It is important that under the action of external DC electric field initially homogeneous cell used to transform to heterogeneous

double-layer cell "thin film of products of viologen reduction – lyotropic liquid crystals". The coloured thin film has a thickness less than 400 nm. Mechanism of resistive photoconversion of dimmers into radical cations under the action of intense laser radiation as dominant optical nonlinearity was proposed for such cells.

Ionic thermotropic liquid crystals of metal-alkanoates can be supercooled to form anisotropic rigid long-living glassy state. Such an anisotropic glass state is characterized by space ordering, which is similar to the mesomorphic smectic ordering. Ionic thermotropic liquid crystals can be first doped with various organic dyes, and then supercooled, forming colored smectic glasses. These novel unusual objects were used as holographic recording media and non-linear optical materials. In the case of homologous series of cobalt alkanoates mesomorphic glasses absorb light in the visible optical diapason (500 – 600 nm). Fundamental physical properties of mesomorphic glasses based on cobalt alkanoates can be tuned not only via changing of the alkanoate anion length, but as well as by varying cation composition for binary and ternary systems.

New nanocomposite materials of metal alkanoates containing semiconductor nanocrystals of cadmium sulfide, which were synthesized in the IGIC NSAU, were investigated from the standpoint of their structure, optical and nonlinear optical properties. By means of x-ray investigation of polycrystalline powders the symmetry and parameters of the crystalline lattice were obtained for two cadmium alkanoates (CdC6 and CdC8) employed as the matrix for the synthesis of CdS nanocrystals. The nanocomposites were established to contain CdS nanocrystals of two crystalline modifications – hexagonal and cubic. Results obtained from the luminescence and excitation spectra of the nano-systems testify for the existence of two principal emission channels in CdS quantum dots: exciton annihilation in the quantum dots and surface localized states.

New materials manifest fast nonlinear optical response accompanied with small thermal effects within the light absorption range. The values of the cubic nonlinear optical susceptibility obtained for different photosensitive centers appeared to be $\chi^{(3)} \sim 4 \cdot 10^{-7} \ldots 10^{-9}$ esu with pico- and nanosecond response times. Relaxation characteristic time of residual thermal holographic gratings was within $\sim 30 \div 100$ µs.

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DISPERSIONS OF CARBON NANOTUBES IN NEMATICS: A PHYSICAL PICTURE OF AGGREGATE FORMATION

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Dispersions of carbon nanotubes (CNTs) in nematic liquid crystalline (LC) matrices are known as promising materials for a number of applications. A major problem is that CNTs in a freshly sonicated dispersion (for concentrations above ~0.05%) rapidly (within minutes or hours) form aggregates resulting in uncontrolled heterogeneity of the material. Several not fully satisfactory ways of avoiding or hindering the aggregate formation have been proposed, but from the physical standpoint, the mechanism of this process remains largely unclear.

A review and generalization is presented of our recent works [1-3], where the process of aggregate formation in dispersions of CNTs in nematic matrix was studied by a number of experimental methods (microscopy, optical transmission and DSC in vicinity of nematic-isotropic phase transition, electrical conductivity and its voltage variation in the region of Freedericks effect, methods of singular optics, etc.). Simple procedures for monitoring the aggregate formation can be proposed on the basis of variations of the measured characteristics with time.

A molecular model simulating interactions of individual CNTs leading to formation of aggregates of the fractal nature was developed. We call such aggregates of anisometric nanoparticles in an anisotropic medium as "S-aggregates", to distinguish them from the "bundles" of substantially different structure often found in LC dispersions of CNTs. Simple relationships involving concentration, aspect ratio, and orientational order parameter of CNTs were obtained. The effective concentration of aggregates was 2-3 orders higher than the initial CNT concentration, with large number of nematic molecules being "captured" in "cavities" and adjacent outer shells of the S-aggregates formed.

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IRREVERSIBLE CHANGES OF RADIATE PARAMETERS OF HIGH POWER LIGHT-EMITTING DIODES AT THE CHANGE OF CURRENT

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By the most perspective sources of luminescence in a visible range and illuminations due to sight of efficiency are the nanoheterostructures of InGaN/GaN. Thus a progress of this direction trend is as an increase of area of epitaxy heterostructures and creation of matrices from the structures of high power light-emitting diodes (LED). Accordingly, swift development of optoelectronics and energy-save technologies requires both comprehensive research of physical properties and operating parameters of heterostructures and application effective methods of nondestruction non-recycling diagnostics and control of degradation.

In this work the spectral and intensity characteristic of high power industrial LED with quantum well are studied.

Electroluminescence intensity of white LED with the colour temperature T_{col} = 3300 K and 5700 K in maximums of blue strip of radiation of the InGaN/GaN structure and strip of the phosphor grows (from something by different inclinations) at the increase of current to J = 1400 mA and then falls. For achievement of big density current (1400-2000 mA) an experiment was conducted at an additional metallic heatsink. Dependences from current of $R(I)$ - relations of the intensities in maximums of injection strip blue electroluminescence InGaN/GaN structure I_{467} and phosphor strip luminescence of the LED1 (I_{583}) and LED2 (I_{564}) $R = I_{583} / I_{467}$ (LED 1) and $R = I_{564} / I_{447}$ (LED 2) have maximum in range 400-500 mA for LED1 (T_{col} = 3300 K) and slump for LED2 (T_{col} = 5700 K).

The sum of intensities of radiation in maximums of two peaks $P = I_{583\ nm}$ + $I_{467\ nm}$ (LED1) $P = I_{564\ nm} + I_{447\ nm}$ (LED 2) is calculated. Evidently, that in initial (total) optical intensity of LEDs with re-absorption photons in the phosphor it is observed maximum at 1050 mA.

It is established that at the increase of current there is growth of the color temperature due to the redistribution of intensities of strips of GaN of structure and phosphor. Thus I_{467nm} and strip of phosphor grows with different in

clinations at the increase of current and then falls, and the white color of radiation of the LED monotones changes from warm on cold. Thus, at the increase of current and at application of heatsink in high power LED based on the GaN with a phosphor there is a change of the color temperature, so change of coordinates of coloured, which enables purposefully to regulate them at the practical using for illumination.

NEW LUMINESCENT PROPERTIES OF ACTIVATED NANOCRYSTALS

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Activated nanocrystals are very attractive materials which could allow tailoring the main stages of a scintillation process (creation of electron-hole pairs and fast thermalization, exciton dynamics, energy transfer and activator luminescence) and reaching high scintillation efficiency.

It is clear today that the spatial confinement in nanocrystals and developed surface result in dramatic changes in the luminescence of activated nanocrystals. The luminescence from the excited Stark components of the split terms of Pr^{3+} ion have been observed due to the quantum confinement in the phonon spectrum of $Y_2SiO_5:Pr^{3+}$ nanocrystal [1]. The decay curve of Pr^{3+} luminescence follows the unusual algebraic low $\sim t^{-0.5}$ that points to the oscillation regime of energy exchange between the localized electronic states of Pr^{3+} ion and the phonon modes of the $Y_2SiO_5:Pr^{3+}$ nanocrystal [2]. The surface stimulated nonuniform tension is the reason of irregular distribution of Pr^{3+} ions within the volume of the $Y_2SiO_5:Pr^{3+}$ nanocrystal that results in specific conditions for the Pr^{3+} luminescence quenching [3,4].

In $Lu_2SiO_5:Ce^{3+}$ nanocrystals of about 5 nm size, the thermoluminescence was not observed [5]. A small volume of nanocrystals and irregular distribution of doped ions enhance the ion and charge interactions and allow the energy storage in $Lu_2SiO_5:Ce^{3+},Yb^{3+}$ and $Lu_2SiO_5:Ce^{3+},Dy^{3+}$ nanocrystals to be controlled [6].

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FERMI LEVEL OF CARRIERS IN MICRO-HULLED STRUCTURE BASED ON HEAT-RESISTANT METALS

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Micro-hulled structure based on metals are widely used in modern nanotechnology, especially when creating high temperature sensors and structural elements based on metal foams. The development of contactless and nondestructive methods for diagnosis and test control parameters of multiply connected matrix base material is a very important and interesting aspect of the application [1]. In a heat-resistant metal with the volume filling defects (VFD) (micro- and nanopores with complex topologies and sizes) it is primarily its strength and electrical and physical characteristics. Almost all rapid methods of such measurements are based on both electrical measurements data and on fundamental functional relationships establishing of the microstructure parameters and the dispersion medium carriers. The influence of a disordered set of volume filling defects (VFD) (micro- and nanopores of complex topology and various sizes) is the unsolved problem on the electronic properties of heat-resistant the micro heterogeneous materials theory. The new statistical "plasma" approach is proposed in this work. This method is based on the modeling statistical concept of the heterogeneous plasma system (HPS) characteristics. The main point of this approach is the concept of an electrically neutral cell. This cell is the smallest area of the electrically inhomogeneous material released by a multiply connected surface Π extreme of instant self-consistent system electric potential [2].

The electronic component statistical equilibrium in volume filling defects of the heat-resistant metals of both nano- and mesoscopic sizes determines the level of electrochemical potential of a homogeneous volume of the sample in any its point. Statistical equilibrium of the electronic component in FVD high-temperature metal nano- and mesoscopic size determines the level of electrochemical potential F of a homogeneous volume of the sample in any its point. Moreover, according to the principle of free energy minimum, F takes the smallest value. Equilibrium distribution of the local density of the electronic component in the matrix base material and VFD satisfies this condition and is determined by solving the effective electrostatic problem in an averaged cell [2]. The external electric field Φ_0 influence on the electrons density distribution in the sample VFD was determined in the computer experiment. The possibility of creating of the sensitive temperature sensors based on heat-resistant metal with nano-VFD was discussed in details .

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SPECTRAL PROPERTIES OF NANOCOMPOSITES BASED ON CADMIUM ALKANOATES WITH SEMICONDUCTOR NANOCRYSTALS CdS

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Novel nanocomposite materials on the base of liquid crystals and mesomorphic glasses of metal alkanoates with semiconductor nanocrystals were synthesized in Institute of general and nonorganic chemistry [1]. In this paper the structure and spectral properties of different nanocomposite materials: (1) $Cd^{2+}(C_7H_{15}COO)^-_2$ + 6 mol.%CdS nanocomposites synthesized by different method, (2) mixture $Cd^{2+}(C_5H_{15}COO)^-_2$ / $Cd^{2+}(C_7H_{15}COO)^-_2$ (mixture components concentrations 50:50 mol%) + 3 mol.%CdS nanocomposites, and (3) $Cd^{2+}(C_5H_{15}COO)^-_2$ + 2 mol.%CdS were obtained. We discuss the obtained absorption, excitation and luminescence spectra of these new nanocomposite materials. With the use of absorption spectra dispersion degree and nanocrystals sizes were obtained (2-4 nm depending on the synthesis conditions). Luminescent properties of cadmium sulfide quantum dots, synthesized on the base of cadmium alkanoates electrostatic layers are being researched for the first time and can serve as a model for studying of luminescent properties in such new structures and influences of medium, surface and polarization effects on them.

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PECULIARITIES OF SPONTANEOUS PARAMETRIC DOWN-CONVERSION MANIFESTATION IN NONLINEAR PHOTONIC CRYSTALS

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An interest to spontaneous parametric down-conversion (SPDC) is caused by the possibility to obtain bi-photons fields consisting of correlated pairs of entangled photons. Along with single crystals the polydomain crystals [1] and crystals with chirped spatial frequency of quadratic susceptibility [2] are also studied as bi-photons sources. This work is devoted to the creation of nonlinear photon crystals on the basis of synthetic opals and to the study of laws in their emission spectra under optical excitation.

Nanodisperse silicon dioxide globules have been received by modified Stöber method [3]. Globules diameter d and distance Λ between (111) planes in various samples were 250–270 nm and 204–220 nm, respectively. Opal infiltration was made by soaking initial samples in a water solution of $Ba(NO_3)_2$, $LiIO_3$ and KH_2PO_4 with the following annealing at temperatures lower than melting ones. Further, some samples were soaked in pure glycerine ($n_D^{20} = 1.4739$) to lower dielectric contrast in nonlinear photonic crystals. Secondary emission in samples was excited by radiation of a 407 nm semiconductor laser with a mean power of 60 mW along z axis parallel [111]. Spectra measured were similar for all infiltrated substances and had a spectral band within a 410 - 650 nm range whose intensity was nonlinearly dependent on substance quantity in opal pores. In emission spectra of samples impregnated with glycerine this band had significant width (≥ 100 nm) and symmetric form with maximum position at 525 nm for $Ba(NO_3)_2$. In spectra of samples without glycerine impregnating the secondary emission intensity decreased within a photon stop-band. In all cases angular distribution of spectral intensity took place. It was fixed as by photographing transmitted radiation as by measuring secondary emission spectra collected at different angles ($1^0 - 5^0$) between excitation and registration directions. In the latter case angular dependences of spectral intensity distribution and intensity maximum position were obtained. Thus, secondary emission observed has been interpreted as SPDC under a quasi-phase-matched conditions $\boldsymbol{k}_{ex} = \boldsymbol{k}_1 + \boldsymbol{k}_2 + m\boldsymbol{q}(z)$, where $q(z) = 2\pi/\Lambda(z)$.

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DYNAMIC SCALING FUNCTION OF NANOLUCTUATION SYSTEM BY USING REFRACTOMETRY DATA

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Equilibration kinetics for inhomogeneous binary methanol-hexane solution under gravity has been studied in the work above the consolute critical temperature, $T > T_c$, by using refractometry technique.

The experimental data of equilibration kinetics of refractive index gradient values $<dn/dz(z,t)>$ have been used to build-up dynamic scaling equation for substance under gravity close to the critical point for temperatures above the critical one $T > T_c$ [1]. Analysis of height and time dependencies behavior of the obtained data $<dn/dz(z,t)>$ has allowed to suppose, that analogous equilibrium properties of substance for certain temperatures $q = (T - T_c)/T_c$ correspond to these nonequilibrium characteristics of solution at different times t.

Proceeding from the qualitatively same time $<dn/dz(z,t)> \sim t^{-x}$ (x » 0.54) and temperature dependencies $<dn/dz(z,t)> \sim q^{-g}$ (g » 5/4) it was proposed the relation between temperature q_i of equilibrium value $<dn/dz(z, \theta t)>$ and time t_i of nonequilibrium values $<dn/dz(z,t)>$: $\theta_i(t_i) = \theta_e(t_i/t_e)x/y = C \cdot t^n_i$. Here t_e is the equilibration time at the temperature q_e; $n = x/g = 0.434$.

On the basis of the obtained data $<dn/dz(z,t)>$ the scaling equations of a nonequilibrium fluid under gravity were suggested:

$$<dn/dz> = \theta^{-\gamma} \bullet f_1(z^*) = t^{-n\gamma} \bullet f^{1"}(z^{*"})$$

Here $f_1(z^*)$ and $f^{1"}(z^{*"})$ are scaling functions of scaling arguments $z^* = z/\theta^{\beta\delta}$ and $z^{*"} = z/t^{n\beta\delta}$ respectively (here g » 5/4; b » 1/3; d » 5 are the critical exponents of the fluctuation theory [2]).

These studies have shown, that kinetics of equilibrium establishment in inhomogeneous nonequilibrium methanol-hexane system under gravity can be described by dynamic scaling equation.

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INFRARED-TO-VISIBLE CONVERSION BY RARE-EARTH IONS IN CRYSTALS WITH METAL NANOPARTICLES

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The effects of metallic nanoparticles (NP) and NP clusters with multi-frequency nanoparticle-plasmon resonance spectra on spectral behavior of atoms located near them are theoretically considered. The results of calculations performed with the framework of quantum and classical electrodynamics are presented both in analytic and graphical forms and can be used for planning experiments and analysis of experimental data.

It is shown that metallic nanoparticles and their nanostructures can be used to control efficiently the rate of spontaneous and induced transitions in atomic systems Thus, an atom located near metallic nanoparticles or their structures (in particular – clusters) haves the rate of stimulated or spontaneous transitions that is ten and hundreds times higher than the rate of these transitions in a free space. The rate of atomic transitions can increase (or slow) by a factor of hundred thousands and even more if nano-bodies from meta-materials (having the negative dielectric constants) are used. The main two new ideas are used in ours work. Firstly, metallic nanostructures with the help of its nanoparticle-plasmon resonances can enhance the rates of ones transitions and inhibited the others. The last can be both the radiating and non-radiating transitions. This gives the opportunity to control kinetics of elementary processes in atomic systems. Secondly, for the first time it is proposed the use of metallic nanostructures for what the nanoparticle-plasmon resonance spectra is in accordance with atomic spectra. These ideas been announced at the international conferences on optical holography and its applications (Kiev, 2004) and on ICONO/LAT (International Conference on Coherent and Nonlinear Optics/ and on Lasers, Applications and Technologies (St. Petersburg, 2005; Programm&Abstracts – IWC3).

TIMES OF LIFE OF FLUCTUATIONS OF ORDER PARAMETER FOR SUPERCRITICAL FLUIDS IN THE GRAVITY FIELD OF THE EARTH

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In connection with the intensive use of unique properties of substance at the critical state in the newest technologies study of these properties of supercritical fluid (SCF) is the urgent task of physics of the condensed state of substance. According to the fluctuation theory of phase transitions the mail structural characteristics of SCF are the size of the fluctuations of the order parameter (correlation length) R_c and the time of its life t_c [1]. Earlier on the basis of the experimental data of molecular scattering of light for the inhomogeneous substances the temperature and field-height dependences of the correlation length $R_c(Dm(z),T)$ of the system have been investigated [2]. On the basis of these data the line of the extremum of temperature dependences of $R_c(Dm(z),T)$ at $Dm(z)=const$ have been founded in the supercritical temperature region. Within the framework the linear model of parametric equation of state the equation of this line of extremum have been calculated [2]. In this work on the basis of obtained $R_c(Dm(z),T)$ data the three-dimensional surface of the times of life $t_c(Dm(z),T) \sim R_c(Dm(z),T)^{3+y}$ of fluctuations of the order parameter has been built for the spatially inhomogeneous systems in the field of gravity of the Earth. The times calculated t_c are close to their values, obtained according to the experimental data of acoustic spectroscopy of liquids at the critical state [3]. It has been shown that on the temperature dependences of $t_c(z,T)$ at $Dm(z)=const$ the line of extremum also appears in the supercritical temperature region. This line of extremum is close to the critical adiabatic curve of substance, which is the line of the maximum probability of fluctuations creation w at the critical state.

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NON-UNIFORM DISTRIBUTION OF DOPED IONS IN Y_2SiO_5: Pr^{3+} AND YVO_4:Er^{3+},Yb^{3+} NANOCRYSTALSDETECTED BY SPECTROSCOPIC TECHNIQUES

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Considerably lower threshold of $^1D_2 ® ^3H_4$ luminescence concentration quenching as compared to correspondent bulk crystals has been revealed for Y_2SiO_5:Pr^{3+} nanocrystals. Analysis of luminescence excitation spectra and decay curves has clearly shown abnormal high quantity of Pr ion pairs in Y_2SiO_5:Pr^{3+} nanocrystal even at negligibly low Pr^{3+} concentration.

Effect of Pr ion pair formation in Y_2SiO_5:Pr^{3+} nanocrystals even at low doped ion concentration was analyzed on the base of surface-induced doped ion segregation theory. Strain gradient determined by nanocrystal surface stimulates the uphill diffusion of doped ions leading to the non-uniform Pr^{3+} distribution, Pr^{3+} pair's formation and as consequence to the low threshold of luminescence concentration quenching. Temperature treatment variation allows us to trace the Pr^{3+} redistribution and to estimate the main diffusion parameters of this process.

Effect of doped ions redistribution observed for Y_2SiO_5:Pr^{3+} nanocrystals must be common for all nanocrystals with different radii of impurity and regular ion. To confirm the generality of this effect the spectra of YVO_4:Er^{3+},Yb^{3+} nanocrystals after different heat treatment were taken. Both Er^{3+} concentration and heat treatment temperature increasing led to similar changes in up-conversion luminescence spectra (increasing of "red-to-green" ratio). So we can suppose that in this case we deal with Er^{3+} temperature dependent segregation manifested itself in redistribution of up-conversion luminescence intensities.

ONE-STAGE ORDERING OF NANOPARTICLES IN POLYMER MATRIX BY THE METHOD OF HOLOGRAPHIC PHOTOPOLYMERIZATION

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Over the last decade, hybrid nanocomposites based on nanoparticles (NP) embedded in a polymer matrix have become the subject of wide scientific research as very promising materials for modern optics, laser physics, and optoelectronics. Creation of polymer–NP periodic structures with a submicron period and different dimensionality (1D, 2D, 3D) opens new possibilities for use of nanocomposites. Specific properties of NP (nonlinearly optical, luminescent, laser) in combination with diffraction properties of periodic structures can be used for creating light-controllable nonlinear diffraction elements, diffraction elements with an ultrahigh spectral dispersion, distributed feedback lasers, in holographic security technologies, etc. Among various methods of obtaining volume spatially periodic structures, holographic photopolymerization is the simplest one-stage method of obtaining 1D, 2D, and 3D structures with a large area and a high degree of faultlessness of the structure.

We present a short overview for results for the development and the investigation of photopolymerizable nanocomposites containing the NP of different nature (metal, metal oxide, semiconductor). The aim of our investigations is to create a maximally universal holographic composition that ensures the formation of periodic structures for NP of different types and is based on known commercially produced monomers.

We propose a holographic nanocomposite that is based on a two-component mixture of commercially produced acrylic monomers with different functionalities, which ensures an efficient spatial ordering of NP in a polymer matrix. We suggest the general approach to the choice of components of a photocurable nanocomposite, and exemplified a high efficiency of the two-monomer system for a number of NP. Using NP of a different nature (TiO_2, ZrO_2, SiO_2, CdSe/ZnS, $LaPO_4$, Au), we have fabricated volume gratings with a period of 0.38–2.1 μm and modulation amplitude of the refractive index of 0.006–0.024, which exceed (in some cases, by nearly an order of magnitude) these parameters obtained for the same NP in composites that involve only one monomer. We suggest a model of formation of polymer–NP periodic structures, discuss particular features of obtained structures, consider the effect of parameters of the interference field (intensity and period) on their characteristics, and give some examples of using obtained periodic structures.

OPTICAL MANIFESTATION OF SELF-ASSOCIATION DYES IN THE NANOSTRUCTURED COMPOSITE THIN FILM

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Creation of material with a controlled response to light has a large potential in different applications due to of the non-contact manipulation of the material. Such processes can induce small changes on the nanoscale that cause a change in the material properties. Applying the technique of sol-gel synthesis we can combine inorganic and organic materials to create composite materials with attractive properties. It is known that dyes molecules in solution can interact electrostatically to form aggregates such as dimmer, which is in turn influenced by several factors, including the concentration, temperature and solvent nature. The work reported here was focused on the aggregative properties of the different dye molecules in spatially separated regions of surfactant-templated mesostructured silicate thin films. In this case, sol-gel synthesis plays a key role, as it provides a low cost tool to obtain mechanically and optically stable organic-inorganic hybrid materials.

We demonstrate results of monitoring of the optical and fluorescence spectra of laser dyes with different nature of the charge state and various concentrations in micelle templated nanosostructured silica films at all stages of its preparation. In addition, the molecular interaction of dyes in normal solvents was studied using visible spectroscopy and luminescence for comparison.

Unusual optical manifold of spatial localization of the dyes and existence of the concentration limit of dyes in micellar space deliberated in the body of mesoporos silica was demonstrated. It is accompanied by the increasing changes of absorption and fluorescence spectra with a formation of ionic pairs of dye and appearance of absorption spectra of the ionic pair due to the centers of monomolecular absorption. In case of excess of the amount of cation dye R6G in a hydrophobic core more than two, formations of excimers and excimer fluorescence excimer fluorescence with the characteristic spectra and lifetime at the simultaneous quenching of the monomolecular fluorescent spectrum is experimentally observed. The more intense and red-shifted peaks in the fluorescence and photoexcitation spectra of R6G in films relative to spectra in amorphous films demonstrate that R6G is incorporated into the micelle body. The manifestation of concentration quenching and aggregation in fluorescence spectra and fluorescence lifetime measurements in mesostructured thin films demonstrate that even large R6G concentrations are incorporated into the micelles interior.

EXCITON TRANSPORT IN AMPHI-PIC J-AGGREGATES FORMED IN POLYMER FILMS

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J-aggregates are luminescent well-ordered nanoassemblies of non-covalently coupled luminophores. Due to high order degree of molecular packing in J-aggregates and strong dipole–dipole interaction between molecules forming the J-aggregate, an electronic excitation is delocalized within a molecular chain forming Frenkel excitons. That explains unique optical properties of J-aggregates: extremely narrow (for organic molecules) spectral width of the absorption band, resonant luminescent, giant oscillator strength, giant optical nonlinearities etc. One of unique properties of J-aggregates is exciton migration over hundreds of monomers. Due to this feature, J-aggregates can be considered as optical antenna for energy delivery purposes.

In the study presented we have determined an exciton migration efficiency in J-aggregates of amphi-PIC (1-methyl-1'-octadecyl-2,2'-cyanine perchlorate) dye, which was formed in polymer films using layer-by-layer (LbL) technique. As exciton traps different polymethine dyes have been used. Exciton migration efficiency was measured using known Stern-Folmer equation of donor luminescence quenching by acceptor. It has been revealed that exciton migration in amphi-PIC J-aggregates is strongly depends on sample preparation method, namely either J-aggregate containing layer forms from monomers or aggregates. Despite on film preparation method exciton transport has been found to be less effective in polymer films comparing solution. The reasons for such difference are discussed.

SCATTERING OF LIGHT THAT COMES THROUGH NEMATIC LIQUID CRYSTAL WITH AGGREGATES OF CARBON NANOTUBES

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We have developed the method of finding the border of perturbed nematic liquid crystal around the carbon nanotubes aggregates by using polarizing microscopy. It is based on the analysis of the intensity distribution and Stokes parameters of light that passes through the sample and comparison of the structure of nanotubes aggregates in nematic and isotropic phases of liquid crystalline matrix.

Nanotubes form clusters of micron size with irregular borders. The interaction of liquid crystal molecules and nanotubes leads to the appearance of transition layer of perturbed nematic, which largely determines the optical characteristics of composites. When concentration of nanotubes is large clusters touch each other and produce a percolation cluster.

The application of an external electric field changes the structure of the transition layer. The inversion walls appear in it.

The investigation of scattering of laser beam that passes through the cell shows that the amplification of scattering during the application to the electric field correlates with the increase of the width of transition layer. The dynamics of speckle and optical singularities in the scattered field has been studied.

SIZE AND TEMPERATURE DEPENDENCE OF THE SURFACE PLASMON RESONANCE IN SILVER NANOPARTICLES

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The dependences of the surface plasmon energy were studied for silver nanoparticles in the size range 11–30 nm and in the temperature interval 293–650 K.

The energy of SPR in silver nanoparticles embedded in silica glass host matrix depends on the size and the temperature of the nanoparticles. Our experiments exhibit the nonlinear red shift of the SPR as the size of the nanoparticles decreases. The increase of the surface scattering rate of the free electrons causes the red shift of the SPR energy as the particle size decreases.

As the temperature of the sample increases, the SPR red shifts. The volume thermal expansion of the nanoparticles leads to red shift of the SPR. As the temperature of the particle increases, the volume of the nanoparticle increases and the density of the free electrons decreases. The lower electron density leads to the lower plasma frequency of the electrons and subsequently to the red shift of the SPR. The red shift of SPR with the increase of temperature is linear for large (25 nm and 30 nm) silver nanoparticles and becomes nonlinear (superlinear) for smaller nanoparticles (17 nm, 11 nm). The nonlinearity of the dependence of SPR energy on temperature becomes stronger for smaller nanoparticles (17 nm, 11 nm). These two effects can be rationalized by the dependence of the coefficient of the volume thermal expansion on the size and temperature of the nanoparticles, The coefficient of the volume thermal expansion increases when the nanoparticle size decreases and with the increase of the temperature of the nanoparticle.

Spill-out and electronic environmental effects were considered as possible mechanisms of the shift of SPR as the temperature and size of the nanoparticles changes. The calculations of the SPR shift caused by these two effects show that it is negligibly small.

NANOPARTICLES INFLUENCE ON THE FREE-RADICAL PROCESSES IN MODEL SYSTEM OF ADRENALINE AUTOOXIDATION

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The ability of nanoparticles (NP) to show antioxidant or pro-oxidant properties is the subject of intensive study [1]. NP similar to superoxide dismutase (SOD) can inactivate highly reactive oxygen species [2].

The ability of NP to change the free-radical processes was studied by the adrenaline autooxidation reaction. Features of the NP influence on free-radical formation processes depending on the form, type and size of NP were studied. Two types of the unmodified particles were used: NP of rare-earth doped orthovanadates with different form-factor, namely – spherical (with an average size of 3 nm), and rod-like (57 × 4.4 nm), and CeO_2 spherical particles with size of 1, 10 and 50 nm. All types of nanoparticles were stabilized by sodium citrate. Nanoparticles concentration (0.2-50 mg/ml) influence on the inactivation of free-radical processes was studied.

It has been observed, that nanoparticles pro-oxidant activity strongly depends on their concentration in solution. CeO_2 particles with size of 1nm and concentration of 2 mg/ml reveal maximal antioxidant activity. At the same time in the case of NP concentration more than 20 mg/ml and less than 0.5 mg/ml, NP have shown pro-oxidant properties. Significant antioxidant effect for solutions with high rare-earth doped orthovanadates concentrations and decrease of this effect under dilution was detected.

Obtained results clearly show that NP influence on the inactivation free-radical processes strongly depends on the nature of NP that can be explained by different interaction mechanisms of free radical with NP surface. Different behaviour of the concentration curves in the case of pro-oxidant or antioxidant effect realization must be considered in the nanomaterial antioxidant activity studies.

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STRUCTURAL PROPERTIES OF SUPERCRITICAL FLUID

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According to the fluctuation theory of phase transitions the main parameter of a substance (the correlation length) unlimitedly increases as the critical point is approached. It leads to the unlimited increase of the compressibility β_T; the heat capacity c_v; the thermal conductivity k of a substance; decrease to zero the diffusion coefficient D; the temperature conductivity coefficient χ. These unique properties of a substance at the critical region (supercritical fluid, SCF) are practically applied in modern technologies.

The purpose of the work is to connect the unique properties of supercritical fluid useful for their practical application with the structure characteristics and the parameters of the equation of state of a substance at the critical region.

The structure characteristics of supercritical fluids have been studied for spatially inhomogeneous systems under gravity near the critical point by the molecular light scattering method. The correlation length, the number of fluctuations of order parameter in one mole of a substance, the total volume of these fluctuations, the density of a substance inside a fluctuation of order parameter have been obtained in the work. The energy of intermolecular interaction inside a fluctuation of order parameter has been also estimated. On the basis of the obtained data the conclusion was made that the unique properties of supercritical fluid, which manifested at its practical application, are caused by the high velocity of the molecules of a substance, $v \geq 10^7$ cm/s, in the process of the creation and break up the fluctuations of order parameter.

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SMALL CLUSTERS OF SI AND GE TERMINATED BY IODINE: MASS SPECTROSCOPY AND COMPUTER SIMULATION

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Small clusters of Si and Ge are the subject of research for many years because of their importance for semiconductor industries. Typically, hydrogen terminated clusters, as conceptually simple structures, have been studied. Another candidate for cluster termination is iodine. It has been shown recently [1] that iodine, like hydrogen, can be used for stable silicon cluster termination. However, no iodine terminated germanium cluster study has been reported yet. Here we present results of our experimental and theoretical studies on germanium iodide clusters, and compare the results with that for silicon iodide ones.

Clusters of Si and Ge iodides were formed by the laser ablation of bulk powder SiI_4 and GeI_4, respectively, in the Bruker Reflex III-T time-of-flight mass spectrometer, equipped with a nitrogen laser (337 nm, 4ns, 300 μJ), and studied in situ. The mass spectra consist of series of main peaks assigned to $Si_nI_{2n+1}^+$ and $Ge_nI_{2n+1}^+$ clusters, respectively, which are followed by weaker peaks. The most abundant clusters in the series are $Si_4I_9^+$ and $Ge_3I_7^+$. For germanium, there are also other peaks assigned to GeI^+, $Ge_2I_3^+$, $Ge_2I_7^+$ clusters. Moreover, the cluster $Ge_2I_3^+$ is the most abundant among all the observed germanium iodide ones.

To elucidate the cluster structures we performed DFT calculations using Firefly software [3]. The calculations on silicon iodide clusters [2] revealed that the abundant clusters are straight chains with iodine bridge in n=1–6, multi-cyclic rings of pentagons in n=7–15, and cages constructed by pentagons and hexagons in n=16–22. Our calculations on germanium iodide clusters confirm the stability of chain structures, like that for silicon, and suggest structures for the clusters that have no silicon iodide equivalent.

Our results show that iodine, like hydrogen, can be used for stable both silicon and germanium cluster termination, and reveal the differences of the clusters. The results can be important for semiconductor industries.

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POROUS III-V SEMICONDUCTORS AS A NANOCOMPOSITES: FAR-INFRARED SPECTROSCOPIC STUDY

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Far-infrared spectral region are very attractive for characterization of porous polar semiconductors because unlike well studied por-Si for polar semiconductor compounds it is the specific region of the Reststrahlen band and also mixed plasmon-phonon mode existence in doped materials. In terms of microstructure porous semiconductor is a typical composite and effective medium approximation (EMA) is absolutely correct in this spectral region where light wavelength is of order of tens micrometers and typical pore diameter is of order of tens nanometers. Systematic theoretical consideration in framework of two basic models of EMA: cavity-Maxwell-Garnett and Bruggeman [1], including porosity and doping influence, isotropic and anisotropic pore disposition, penetration depth is presented.

Porous layers were obtained by electrochemical etching of _n_-type GaAs, InP and GaP single crystals in water and ethanol solutions of the HF, HCl and H_2SO_4 acids correspondently, mainly in the galvanostatic regime. Free charge carriers concentration was in wide region 10^{16} - 10^{18} cm^{-3}, this makes it possible to investigate pure phonon and mixed plasmon-phonon modes. SEM measurements show that diameter of pores is in the range 50 - 200 nm and porous layer thickness is in the range 5- 90 mm depending on etching conditions. Optical studies include near-normal reflectance and ATR measurements including surface polariton (SP) excitation regime in the 20–50 μm spectral region. The experimental spectra of porous materials clearly exhibit different changes in comparison of the bulk one: shape modification of the Reststrahlen band in the reflectance spectra and shift, splitting or disappearance of the minima corresponding to SP excitation in the ATR spectra.

In conclusion, the EMA can be efficiently applied for studies of porous A^3B^5 semiconductor media in the far-infrared region including the existence range of surface phonon and plasmon-phonon polaritons. At the same time, the specific effective medium model to be used is dictated by the symmetry and microstructure of the porous medium under study. As shown theoretically and supported by experiment, SP spectroscopy shows much promise for porous composite medium characterization, since SPs are very sensitive to the essential parameters of porous semiconductor layers (porosity, symmetry, free carrier concentration, thickness, etc.).

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RAMAN STUDY OF MONOCLINIC TO TETRAGONAL PHASE TRANSITION IN ZIRCONIA AND HAFNIA

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Zirconia (ZrO_2) and Hafnia (HfO_2) are promising materials for creation of piezo- and constructional ceramics, bioceramics, materials for solid electrolytes, optical materials and for some other applications. The significant attention to the materials on the basis of zirconia and hufnia is caused by their unique combination of properties such as high strength and fracture toughness, resistance to effect of aggressive chemical conditions, low thermal conductivity, and special electro-physical properties. These properties essentially depend on the crystal structure of the mentioned materials. The application of Raman spectroscopy considerably expands the possibilities of study of the material crystal structure, the phase transformation peculiarities, the quantum size effect, compositional effects, the material evolution with treatment.

In present work we study Raman spectra of two polymorph modifications of zirconia and hafnia – monoclinic and tetragonal. The nanocrystalline powders and pressed pellets prepared by means of different technological conditions were investigated. Nanocrystalline powders and polycrystalline samples were obtained by the method of the high-temperature hydrothermal synthesis which allows obtaining more homogeneous powders with the narrow size particle distribution. The control of phase composition of samples has been carried out by X-ray phase analysis. Raman spectra were obtained using double grating spectrometer DFS-24 in photon counting mode in backscattering geometry at room temperature.

Observed Raman spectra contain all fundamental optical modes, as predicted by the group theoretical analysis for monoclinic and tetragonal modifications, both for powders and polycrystalline pressed pellets of the same composition. The band intensity relationship depends on the type of sample.

The full interpretation of Raman spectra of materials under study have been done using the obtained forms of the fundamental vibrations. The correlation between phonon modes of lattices of both polymorph modifications has been discussed.

MODIFICATION OF OPTICAL PROPERTIES OF POROUS A^{III}B^{V} LAYERS PRODUCED BY ANODIC ETCHING

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Porous (chemical, electrochemical) layers of A^{III}B^{V} semiconductors are usually used in photodetectors and various physical sensors to reduce optical losses and to increase sensitivity of materials with huge specific surface area.

The morphology and optical properties of the porous layers on GaAs and InP single crystals were investigated by atomic force microscopy (AFM) and scanning electron microscopy (SEM), monochromatic multi-angle-of-incidence (MAI) ellipsometry, photoluminescence (PL), Raman scattering (RS).

In this work the porous layers on the n-type GaAs (0.5 - 2) x 10^{18} cm^{-3} and n-type InP ($10^{18} – 10^{19}$) cm^{-3} wafers were prepared by electrochemical etching in HF:H$_2$O and HCl solutions, respectively. Two-layer structure of porous layers was confirmed by AFM and SEM methods. The top layer consists of oxides and reaction products. It also contains some GaAs or InP nanocrystals. The optical parameters, the reflection index, n and extinction coefficient, k, have been determined by MAI ellipsometry. It has been shown by the example of porous GaAs layer that the porous layer on single crystal can be presented as semi-infinite medium with optical parameters of porous layer and some oxide overlayer. This approach confirms the surface morphology of studied porous A^{III}B^{V} materials. Photoluminescence spectra of investigated materials at room and low (77 and 2 K) temperatures have shown the change of the surface recombination velocity and quantum confinement effect for excitons in GaAs and InP. PL from porous GaAs in visible spectral region can be caused by transitions associated with impurities and defects in oxide layer. Raman spectra of porous GaAs and InP samples have been compared. They have shown similar peculiarities. In porous layers comparatively with the flat surfaces the TO, LO phonon modes in RS spectra are of the same order of intensity due to the surface enhanced scattering and the violation of the selection rules for the TO mode in (100) geometry. The surface phonon lines and the quantum confinement effect for phonons were identified reliably in some samples of porous GaAs. The size of nanocrystals in the porous GaAs and InP was estimated by RS, PL and SEM/AFM. An application of porous A^{III}B^{V} layers as antireflection coating in photodevices and as sensitive area in optochemical sensors has been also discussed.

SYNTHESIS AND OPTICAL PROPERTIES OF TRANSPARENT NANOCOMPOSITES MATERIALS BASED ON CdS, ZnS, CdZnS/PMMA

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In the last time the polymers of acrylic row, in particular polymethyl-methacrylate imobiolized in his volume nanoparticles of semiconductors groups of $A^{II}B^{VI}$, find a wide application in the different fields of science and engineering, goods on their basis it is possible to take to organo-neorganical multifunctional optically transparent materials. Such composites, as rules get, by either the sorption of precursors in the porous previously obtained polymeric matrix, and then directly precipitate nanoparticles in the pores of these materials in the process of impregnation of him in solution precipitator or initially obtained nanoparticles of semiconductors by a micro emulsion method, and then carry them in medium methyl methacrylate (MMA) with his following photopolymerization. The lack of these methods is that extremely difficult to obtain the even distributing of nanoparticles in the volume of polymeric matrix, besides in the case of micro emulsion method evaporation of original solvent for the transfer of nanoparticles in medium of monomer, that not always it is possible to carry out without the change of properties of particles of semiconductors and polymeric block composite on the whole. The direct synthesis of nanoparticles of semiconductors in such monomers was impossible until recent times, because of low permittivity of MMA. In similar environments dissolution, both organic and inorganic salts, with a high or low concentration is difficult and on some case not in the least possible.

It is shown, that using salt of trifluoroacetate specifically cadmium, zinc and their mixture as initial precursors able for lights dissolution in MMA allowed to realize one-stage dimensionally controlled synthesis of chalcogenide nanoparticles such as CdS, ZnS, CdZnS directly in monomer, and following photo- or thermo polymerization gets for obtaining hybrid optically active material with even distributing of nanoparticles within polymeric composite, and size of synthesized particles gives on the phase of synthesis and varies from 4 to 10 nm. It is shown, that properties of their composites on the whole and straight depend on size of synthesized particles.

SHAPE AND LOCATION OF CHARGE WAVES IN IONIC POLYMETHINE SYSTEMS IN ELECTRIC FIELD

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A quantum-chemical investigation of the charge distribution and molecular geometry in ions of linear conjugated molecules in electric field has been carried out. It was shown by quantum field theory that a charge in the collective π-electronic system is autolocalized and forms both charge and bond length solitonic-like waves. Introducing the donor groups generates additional waves at the conjugated chain ends, what causes the symmetry breaking in the long polymethine-cations. In the short molecules, the contribution of the terminal groups becomes predominante. Such character of the charge distribution received by quantum field theory calculations is confirmed experimentally by the NMR spectra.

Keywords: linear conjugated systems, polymethine dyes, quantum-chemical calculations, quantum field theory, charge waves, bond length waves, soliton, NMR spectra.

STRUCTURE AND ELECTROLUMINESCENT PROPERTIES OF TETRACENE THIN LAYERS DEPOSITED ON Au ISLAND FILMS

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Lately tetracene has attracted much interest in connection with development of organic light-emitting field-effect transistors [1]. Earlier we found out a possibility to fabricate planar light-emitting systems consisting of Au nanoislands and organic luminophores, and showed that the light emission from such nanostructures features emission spectra from both metal nano-islands and luminophore molecules [2].

In the present work we report on a systematic study of molecular structure, morphology and electroluminescent properties of tetracene thin layers deposited in vacuum on Au island films. FTIR absorption spectra of the obtained samples were measured at room temperature (Bruker IFS-88, 2cm^{-1} resolution, 64 scans) and showed pronounced changes in position and intensity for major absorption bands compared to those of polycrystalline tetracene. The observed changes indicate strong interaction of adsorbed tetracene molecules with Au surface. Scanning tunneling microscopy studies revealed an amorphous structure of the deposited tetracene layers. It was also found that local current-voltage characteristics (CVCs) of the obtained tetracene films with a thickness of about 100 nm have a pronounced non-symmetric shape.

For electroluminescent studies, a planar gap-type cell was fabricated. The cell consists of two conducting metal strips deposited on a dielectric substrate and separated with a narrow (~10 μm) gap. By UHV deposition method, the gap is covered with Au nanoislands and then with a tetracene thin layer. Upon application of ~5 V electric voltage corresponding to a super-linear region of CVC, a photonic emission from the nanostructure is observed. Monotonic increase of light emission with applied voltage is accompanied by flashes correlating with jump-like increase and decrease of conduction current. These results show that polycyclic aromatic hydrocarbons can be prospective materials for application in planar light-emitting structures based on metal nano-islands.

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EFFECT OF TEMPERATURE ON STRUCTURE OF NANOHYBRID FORMED WITH CARBON NANOTUBE AND POLYNUCLEOTIDES

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Recent revolutionary progress in synthesis and characterization of single-walled carbon nanotubes (SWNT) has demonstrated the enormous potential for the development of new devices with unique capabilities. Furthermore, biological molecules (especially, nucleic acids) are easily combined with SWNT, forming multifunctional materials with new properties. However, the mechanism of this process is still not well understood.

The present study was aimed at revealing of changes in physical and optical characteristics of single-stranded nucleic acids (NAs) and SWNT owing to the formation of a complex between them. Aqueous suspensions of nanohybrids have been investigated by differential UV-visible absorption spectroscopy in the temperature range from 20 ^{0}C to 90 ^{0}C. Heating NAs-SWNT hybrid can lead to changes in its light absorption, which reflect the conformational change of the adsorbed molecule, as well as the change in SWNT absorbance at disruption of base-stacking interaction within NAs and with SWNT surface, respectively.

According to measurements at 20 ^{0}C, homopolymer adsorption onto the nanotube is followed with changes in optical characteristics both of the polymer and SWNT, being the result of p-p-stacking interaction of the polymer with the tube surface. Attenuation of the light absorption intensity was observed in the range of (44000-38000) cm^{-1} where the polymer and the tube absorb and in the range of only the nanotubes absorption ((35000-27000) cm^{-1}). It was revealed that upon poly(rA) wrapping on nanotubes a significant part of its bases keeps self-stacking while upon adsorption a more rigid poly(rC) is disordered almost completely. The temperature increase to 90 ^{0}C does not result noticeable nanotube precipitation. On melting curves of polynucleotides the features are revealed which can be explained by a re-orientation of these polymers on the nanotube with the heating that provides the optimal π-π -stacking of nitrogen bases with the carbon surface. The complexes formed by a flexible disordered poly(rI) and nanotubes show a lower stability. With increasing temperature to 90 ^{0}C the nanotube precipitation (about 12% of SWNT) was observed, indicating that complex degradation occurs through a loss of π-interaction. This assumption is confirmed by a hyperchromicity of nanotube absorption.

The experimental data are explained by results of molecular dynamics simulation of NAs-SWNT hybrids.

LOW-TEMPERATURE RAMAN SPECTROSCOPY OF DNA-WRAPPED SINGLE-WALLED CARBON NANOTUBE FILMS

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A single-walled carbon nanotube (SWNT) is a quasi-one-dimensional crystal characterized with unique physical and chemical properties, which can be used in various fields of nanotechnology. Under ordinary conditions, because of the strong van der Waals interaction between individual nanotubes, they form bundles. For practical applications it is important to obtain isolated SWNTs. Bundles can be separated in the water medium by means of ultrasonic dispersion in the presence of a surfactant or water soluble polymers, for example, DNA. This polymer wraps around SWNT and prevents nanotubes from re-aggregating into bundles after the ultrasonic treatment. Besides isolated SWNTs in aqueous suspension, it is necessary to obtain individual nanotubes in the composite film. In connection with this problem, a question of the environment affect on SWNTs physical properties is topical now.

Herein, we report results of our work on studying the environment effect on Raman spectra of HiPCO SWNTs in a film with DNA at 5 and 295 K. Resonance Raman (RR) spectra of DNA-wrapped single-walled carbon nanotube films were studied in the range of radial-breathing (RBM) in (175–320 cm^{-1}) and tangential (G) (1520–1625 cm^{-1}) modes. The carbon nanotube-DNA interaction results in the following changes in RR spectrum of this sample, relatively to the spectrum of nanotubes in bundles: increasing of the integral intensity of RBM bands, redistribution of intensities between the bands, which can be partly explained by transformation of resonance conditions, G band is upshifted, and the intensity of the asymmetric band of the low-frequency component of this band weakens in the film. The temperature lowering from 295 to 5 K is accompanied by the upshift of RBM bands, the magnitude of which is higher for metallic nanotubes than that for semiconducting ones. Upon the temperature lowering from 295 to 5 K, the upshift of bands attributed to G mode is observed for two samples but its magnitude is different for metallic and semiconducting nanotubes. It should be noted that the spectral shift value between the high-frequency component of G band peaks of two samples at 5 K retains the same as it was observed at 295 K. In general, it can be concluded that temperature changes observed in RR spectra of SWNT:DNA film and nanotubes in bundles are similar. It results from the fact that the strong interaction between tubes in bundles is replaced with a rather strong SWNT interaction with the polymer.

SEIRA AND ENHANCED IMAGING OF LIVING CELLS ON THE GOLD NANOSTRUCTURED SURFACE.

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A new method for imaging, structural study and cultivation of cells based on the effect of the enhancement of optical signals from biomolecules near the nanostructured rough gold surface is proposed. The SEIRA (surface enhanced infrared spectroscopy) and confocal microscopy experiments were done on culture of SPEV (porcine embryonic kidney epithelium transplantable line) cells cultivated and adsorbed on the gold support.

The first SEIRA spectra have been registered from monolayer of the SPEV cells with better resolution than those for monolayer of protein or other biopolymers. They showed a low frequency shift about 2-7 cm^{-1} of the most IR vibrations for cells cultivated on the rough gold in comparison with those for adsorbed cells from suspension on the same substrate. Factor of enhancement was equalled to 15-30. Then we visualised SPEV sells on the rough gold support and got contrast image in laser fluorescence mode.

Confocal imaging was done by a Carl Zeiss LSM-510 META confocal laser scanning microscope with Plan-Achromat 63x/1.4 Oil DIC oil immersion objective in Multi Track mode. The FTIR spectra were collected in the 400–7000 cm^{-1} region with an IFS 66 Bruker instrument with resolution of 0.5 cm^{-1} and precision of wavenumber definition not less than 0.01 cm^{-1}. SPEV cells were cultured in plastic flasks in DMEM (Sigma) medium.

This approach could open new possibility for imaging of living cells, cells in vivo without staining and without labelling. Fluorescence from the rough gold have been registered for three laser excitation in confocal microscopy. The plasmonic effect responsible for our findings is discussed.

DEEP TRAP LEVELS IN InGaAs/GaAs QUANTUM DOT STRUCTURES

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Deep electron traps in InGaAs/GaAs quantum dot (QD) structures, which largely affect the transport of charge carriers and photoconductivity of the system were identified by thermally stimulated conductivity (TSC) technique. The discrete values of deep level depth below GaAs conduction band at 0.16 eV, 0.22 eV, and 0.35 eV were obtained from analysis of TSC curves shape after excitation with quanta energy $hv = 0.9$ eV, 1.2 eV and 1.6 eV.

Observation of TSC curve peaks with maximums T_m near 90 K, 106 K, and 187 K pointed to existence of tree deep electronic states at least, which are localized at GaAs intermediate layers in the vicinity of QDs.

The shape of TSC curve depends on quanta energy. After exciting of structures by photons with energy outside the PL band, it was impossible to observe the second TSC peak (state at E_c – 0.22 eV) near 106 K. Peaks near 90 K (state at E_c – 0.16 eV) and 187 K (state at E_c – 0.35 eV) were observed only after excitation by hv of 0.9 eV and 1.6 eV. This means that the second peak is associated with deep recombination center located outside the QD. The state at E_c – 0.22 eV is shown to be related to the recombination centre, which can hold non-equilibrium holes over a long period of time on condition that non-equilibrium holes localized by quantum states of QDs. During long-term electron storage in the vicinity of QDs, the electron trapped at E_c – 0.16 eV level are recaptured by deeper and remote spatially E_c – 0.22 eV level, which causes TSC peak observation at 106 K. With respect to spatial localization and the physical nature of deep-level traps, we can assume that deep levels E_c - 0.16 eV and E_c - 0.22 eV may be assigned to $In_{1-x}Ga_xAs$-GaAs interface defects.

Presence of recapturing is illustrated by peak shifting at different heating rates. Peaks shift to higher temperatures with increasing of heating rates, while maximum values of the conductivity are growing up. Data obtained at different heating rates allow us also to calculate the depth of the deepest trap 0.35 eV, which is responsible for observation of the TSC peak near T_m = 187 K. Such levels may be assigned to EL6 traps in GaAs.

The study shows that level with depth of 0.16 eV is effective electron trap, which provides crossing of lateral conductivity to high-resistance mode, and therefore causes a high value of photocurrent sensitivity about 3 A/W at 77 K with excitation by interband transitions in QDs. The charge density of electrons captured by E_c – 0.16 eV level was determined to be 2×10^{-6} C/cm^2 at 77 K, which induces electric field $\sim 10^5$ V/cm in the vicinity of QDs.

SPECTRAL INVESTIGATIONS OF MEROCYANINE DYESIN MICELLAR SYSTEMS WITH SURFACE-ACTIVE COMPOUNDS

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This paper investigates bistable merocyanine dyes (oxynitrostiril tetrahydro-fenantridine (SF)) with photo and thermochromic properties. These compounds are sensitive to the characteristics of the environment.

To study the dependence on the environment of properties of SF dye compositions the solvents with surface-active substances (SAS) were used. It was revealed that at certain concentrations of surfactant in such compositions the self-organization of molecules and formation of supramolecular nanostructures are going on. The formation of micelles is accompanied by formation of local areas, which in general differs in characteristics from the environment. Spectral studies were conducted for different concentrations of dye and SAS and for the different ratio of components.

Absorption spectra of dye solutions in chloroform without SAS consist of broad bands in the ranges of $\lambda_{max} = 320$ nm, $\lambda_{max} = 410$ nm, $\lambda_{max} = 610$ nm, and luminescence spectra have bands in the range of $\lambda_{max} = 490$ nm and $\lambda_{max} = 700$ nm, respectively and caused by emission of dye's monomers and excimers.

Premicelle concentrations of SAS do not influence the spectral characteristics of dyes. It means that SF does not form with SAS any chemical compounds or complexes.

The increasing of monomer and extinction of excimer luminescence of the dye is observed after reaching the concentrations of SAS micelle-creation. At the same time, the spectra of absorption remain practically unchanged. These experimental results testify that the creation of micelles impedes SF intermolecular interaction as well as the possibility of inclusion of the dye molecules to the micelle.

Further increasing of SAS concentration over the critical level of micelle-creation leads to considerable changes in spectra of absorption and luminecence and is accompanied with decolouration of dyes. The bands of SF merocyanine form disappears while the bands of SF spirane form increse in the spectra: absorption $\lambda_{max} = 330$ nm, luminecence $\lambda_{max} = 500$ nm. The existance of isobestic point confirms the shift of balance to the colorless form of SF in certain concentrations. The experemental results could be explained by fixation of molecule of the dye in the micelles, where the local environment with reduced polarity is established as the consequence of pecularities of micellar structures with inward directed non-polar tails of SAS molecules.

SYNTHESIS AND CHARACTERIZATION OF ORGANIC DYE-DOPED SILICA NANOPARTICLES

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In the last ten years, significant advances have led to a large variety of labelling reagents based on nanomaterials with controlled size and shape. These materials represent an exciting and often more effective alternative to the use of organic fluorophores. Such nanomaterials show many unique properties that are not observed in the bulk materials. Dye-doped silica nanoparticles possess significant advantages over single dye labeling. They are made of thousands of organic or inorganic dye molecules doped inside a silica that protects dye from the surrounding environment, increases photostability, and provides fluorescent signal enhancement.

The work presents experimental results on synthesis of silica nanoparticles doped with polymethine dye DiI and studding their luminescent properties. Silica nanoparticles were synthesized by the modified Stöber method and characterized by TEM. The influence of reactant concentrations (ammonium hydroxide and TEOS) on SiO_2 nanoparticle size and size distribution has been examined. Dye molecules were encapsulated into SiO_2 matrix by three different methods: during the nanoparticle synthesis, by the SiO_2 nanoparticles impregnation with the dye and using layer-by-layer self-assembly technique. Comparison analysis of fluorescence spectra, photostability and dye-leakage ability for three different types of dye-doped silica nanoparticles have been done.

PLASMON-ASSISTED RARE EARTH FLUORESCENCE FROM SOL-GEL MATERIALS

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Sol-gel synthesis of oxide matrices doped with rare earth ions can provide economic luminescent materials for photonics, lighting and displays. They permit incorporation of noble metal ions and nanoparticles for plasmonic enhancement of the impurity fluorescence. But the efficiency of energy transfer from noble metal dopants to the fluorophore not exceeded 20-40 % till recently [1].

Sol-gel TiO_2 films activated by Sm^{3+} ions and co-doped by silver particles described here demonstrate up to 20 times enhancement in fluorescence. Strengthening of Sm^{3+} absorption by plasmons localized in silver particles is considered as a reason of such enhanced emission [2]. Sol-gel TiO_2:Sm^{3+} films deposited on thin (50 nm) gold layers allow tuning of spectral distribution and polarization of Sm^{3+} emission. Such effect is due to coupling of fluorescence with surface plasmon waves induced in gold layer.

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STRUCTURAL DEFECTS INFLUENCE ON OPTICAL PROPERTIES OF FILM OPALS

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Interest to opal films is caused by an opportunity of manufacturing on their basis optical splitters, filters, integrated optical circuits, memories, optical sensors and etc.

The purpose of the present work was grew film of opal on a basis of silicon dioxide globules and investigation structural disorders influences on their optical properties.

Synthesis of silicon dioxide globules was carried out by modified Stober method [1]. Opal films were grown by vertical pulling of quartz or glass substrate from suspension of nanodisperse silica globules with middle size of about $D = 240$ nm. Speed of pulling was of about 100 nm/s. In this case, under action of forces of a surface tension of particle suspension, globules were stacked in a uniform layer. Such method of film creation as shows experience, is most effective and occupies

much less time than method of film growing in a region of moving meniscus by evaporation of a liquid from suspension [2]. The samples received thus were dried up during day at room temperature with the subsequent annealing at T = 480 ^{0}C.

Diffraction of laser radiation with $\lambda = 640$ nm at the relation $D/\lambda = 0.37$ (near lower edge of photonic stop-band) on the prepared opal film samples was observed, while authors of work [3] observed diffraction patterns in the range from $D/\lambda=1.07$ to $D/\lambda=2.10$ that corresponds to photonic forbidden band of higher orders. Character of distribution and brightness of diffraction reflexes was various in various sites of a sample that testify to polydomain structures of film. Reflection spectra from various sites (size $\sim 200 - 300$ μ) of film with use of specially developed optical probe are measured by double monochromator DFS-12. The various character of spectral distribution caused by influence of point defects, "strips of growth" and structural disorders in various sites of a sample is established.

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MICROSTRUCTURAL, RHEOLOGICAL, AND CONDUCTOMETRIC STUDIES OF MULTIWALLED CARBON NANOTUBE SUSPENSIONS IN GLYCEROL

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Optical microscopy studies of electrical conductivity and rheological properties (in the cone-plate geometry) of glycerol suspensions filled with multiwalled carbon nanotubes (MWCNTs) have been fulfilled [1]. The researches were carried out in the intervals of temperature T=283÷333 K and MWCNT concentration C=0÷l wt%. MWCNTs in glycerol are demonstrated to have a strong tendency toward the aggregation, so that "primary" MWCNT aggregates persist even after the intensive ultrasound homogenization. Typical percolation phenomena accompanied by an enhancement of the electrical conductivity and the viscosity are observed at an increase of the MWCNT concentration. The concentration percolation threshold is identified at $C=C_p \approx 0.1$ wt%, and the scaling behavior in a vicinity of the percolation threshold is found to be characterized by the conductivity exponent t=2.7±0.3, which is somewhat higher than a value typical of the random percolation problem. The introduction of MWCNTs in glycerol resulted in the appearance of thixotropic behavior related to the fracture of MWCNT aggregates under shear. An anomalous rheological behavior is observed at a high MWCNT concentration, C=1 wt%, which testifies to the destruction of the H-bond network in glycerol induced by MWCNTs. The dependences of the activation energies of the ionic electric conductivity and a viscous flow on the MWCNT concentration are estimated.

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UV ABSORPTION OF NANOSTRUCTURED TITANIUM DIOXIDE DOPED WITH TRANSITION METAL CATIONS

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Titanium dioxide, TiO_2, is attracting much interest for its unique properties, such as high dielectric constant, high refractivity, ferromagnetic phase above room temperature, photocatalytic activity etc. But still, wide technological usage of TiO_2 as solar cells and photocatalysis is impaired by its large band gap (3 eV for rutile and 3.2 eV for anatase), which requires UV irradiation. Many attempts have been made to modify the physical, chemical and optical properties by doping TiO_2 with different metal cations. New physical and chemical properties can thus be imparted to nanostructured TiO_2 depending on the synthesis procedure and dopant type and content. These materials seems to possess unique optical and photocatalytic properties, as well as it might be a perspective material for solar energy conversion.

In the present work, a comparative study of UV optical absorption of anatase (A) and rutile (R) polydisperse nanopowdered TiO_2 doped with different transition metal ions Cu^{2+}, Fe^{2+}, Co^{2+}, and Cr^{3+} was performed. The doped anatase samples have revealed an increased optical absorption and significant red spectral shift of the absorption edge, whereas rutile samples have no such shift of the absorption edge. The doping effect in the absorption of rutile is observed only in the range 3.0-4.5 eV, whereas the absorption of doped anatase differs from pure anatase in the range 3.0-5.5 eV. The samples were characterized by XRD, TEM-EDX, UV-spectroscopy, and Fourier transform (FT) Raman and IR spectroscopic techniques. Correlation between the structure and optical properties is discussed.

EFFECT OF IMPURITIES ON BAND GAP AND PHOTOCATALITYC PROPERTIES OF NANOSTRUCTURED ANATASE AND RUTILE

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Nanocrystalline titanium dioxide (TiO_2) is a photoactive semiconductor material with multifunctional properties including high dielectric constant, high refractive index, high optical absorbance in the ultraviolet and transparency in the visible spectrum, which are widely used in photocatalysis, photovoltaic cells, photosensors and photonic crystals [1,2]. However, the large band gap of TiO_2 (3.2 eV for anatase, 3.0 eV for rutile) allows its activation only in the UV light (wavelengths $\lambda < 400$ nm) that limits possible applications, for instance, in photocatalysis under the natural solar irradiation.

In this work, the values of the band gaps for direct (E_{gd}) and indirect (E_{gi}) transitions for the studied anatase samples are obtained. For pure polydisperse anatase, the direct band gap value is shown to be E_{gd}= 3.25 eV. Our values of the direct band gaps for the doped anatase correlate well with the literature data for anatase with similar impurity cation concentration and particle size.

It is found that, as compared with pure rutile, the band gap in the doped rutile does not change, whereas for the doped anatase it decreases, and most of all for A/Cr and A/Fe samples. It is shown that the large amount of transition element impurities in the doped TiO_2 samples create additional recombination centers for photogenerated electrons and holes, which cause the inhibition of photocatalytic activity. It is found that the improvement of photocatalytic activity of the doped TiO_2 in the reaction of organic dye safranine destruction is most pronounced for the anatase samples as following: A/Fe>A/Cu>A/Co>A. It correlates with the relative intensity of photoabsorption of doped anatase at the 4.0-5.5 eV. In the case of rutile samples, the doping effect leads to the inhibition of the photocatalytic activity as following: R/Fe<R/Cr<R/Cu<R/Co<R.

PROGNOSTIC OF DEGRADATION OF EL-SPECTRUM HIGH POWER LED ON THE BASIS OF InGaN/GaN NANOHETEROSTRUCTURES WITH QUANTUM WELL

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In work the question of working out of new methods of an establishment and forecasting of duration of term of maintenance of operational parametres of high power commercial light-emitting diodes (LED) on the basis of InGaN/GaN nanoheterostructures with quantum well on the basis of complex examination of their performances the acoustics emission (AE) method and the spectrographic analysis is considered.

It is known that operation LED at excess of the recommended temperature considerably reduces the guaranteed term of work because of acceleration of processes of a defect formation in nanostructure. It influences also character of dependence $I(J)$ powers of radiation - electroluminescence (EL) I from supply current J and an energy distribution in its radiation spectrum.

Originally, the AE-method was erected maximum allowed current and temperature of operation LED. Because of the analysis of dynamics of intensity and peak distribution of AE-signals, the deduction about criticality and intensity of processes of formation of defects, reliability and expediency of magnitude of a loading, and its subsequent magnification became.

The subsequent measuring were lead at the stand of a spectrograph with a ruler of photodetectors (time of recording of a spectrum less than 10 ms), a measuring instrument of integrated power of radiation (sensitivity practically does not depend on a radiation wave length in a range 250 - 3000 nanometers), with spectroscopic not selective thermoelectric detector, a control system and the control of temperature LED.

The algorithm of processing of results is offered allows to build power distribution in a spectrum of the EL, and also to find out differences in $I(J)$ for LED different power at various temperatures (for example, at 250 °C and 550 °C). Diagram's $I(J)$ are well approximated by multinominals of the second degree. It is revealed that type LED coefficients of multinominals depend on temperature.

The registered changes in spectrums of radiation LED at various temperatures allow doing quantitative assessments of subjective perception as changes of color of radiation (taking into account spectroscopic sensitivity of an eye of the person).

ABNORMAL LOW LINEWIDTH TEMPERATURE BROADENING OBSERVED FOR YVO$_4$:Eu NANOCRYSTALS

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Since the spectral lines temperature broadening are determined by phonon scattering on the impurity centre modification of phonon spectrum can affect the temperature broadening suppression. So, by controlling of nanocrystal size and "nanocrystal - environment" interface the effect of "cluster freezing" – abnormal weak spectral lines temperature broadening up to room temperatures – can be achieved.

Spectral lines of impurity ions in YVO$_4$:Eu^{3+} nanocrystals remain abnormal narrow ($\sim$10 cm^{-1}) even at the room temperature, while for the bulk crystals the average linewidth at the room temperature is $\sim$70 cm^{-1}. This narrowness of spectral lines can be clearly explained by manifestation of phonon spectrum depletion in nanocrystals. Linewidth temperature dependences obtained for nanocrystals with different size exhibit strong dependence of spectral line width from the size of nanocrystal and differs from bulk crystal (Fig.1).
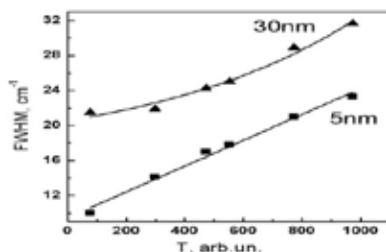
Fig.1

Decreasing of crystal size up to few nanometers manifests itself in significant modification of phonon density of states $\rho(\omega)$. Obtained data are in good agreement with equation for spectral linewidth (1), where $\rho(\omega)$ is phonon density of states corresponding to nanocrystal size.

$$\gamma(T) = \int\limits_0^\infty \frac{d\omega}{2\pi} \ln\left\{1 + W^2 \cdot \rho^2(\omega) \cdot sh^{-2}(\hbar\omega/kT)\right\} \text{ (1)}$$

ON THE POSSIBILITY OF NANOFLUIDS USING AS A COOLANT

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The heat-transfer properties of "water-nanofluids" liquid system, which contains high-purity single-walled nanotubes SWCNTs, have been investigated [1]. It was found that the relation of heat conductivity factor between the nano-structuring liquid and the classical one has linear dependency in concentration range of C=0÷0.3 mg/l (see Figure).
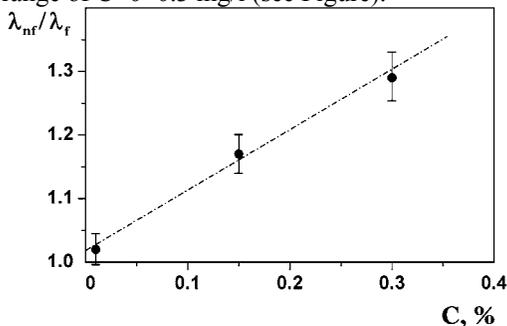
Figure: λ_{nf}/λ_f as a function of concentration C for liquid system "water-nanotubes" (λ_{nf} is the nanofluids thermal conductivity coefficient and λ_f is the classic liquid one).

For the reason of performed experiment we propose the possibility of nanofluids using as a coolant.

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RESONANCE PHENOMENA IN RAMAN SPECTROSCOPY OF FILMS OBTAINED FROM C$_{60}$ MOLECULAR BEAMS

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At ambient conditions, fullerene C$_{60}$ forms nearly ideal molecular crystals with the molecules bound by Van der Waals interactions. In the last years, a new carbon structure (carbon like and diamond like) has been prepared from fullerene C$_{60}$ under high pressures and temperatures. These materials show different electrical and optical behaviours, according to their structure, depending on several parameters in each production method. In this work, investigation results of Raman spectra in obtained from C$_{60}$ molecular beams films been presented. Films were produced from C$_{60}$ fullerene powder by sublimation in vacuum on Si and quartz unheated substrates. Raman spectra C$_{60}$ films display lines peaked at 1426, 1470 and 1578 cm^{-1}. It has been reveal itself that C$_{60}$ molecules decomposed and that new carbon structures (graphite like and diamond like) form in the films depending on the C$_{60}$ beam energy. We have carried a study of this films Raman spectra, by measuring it at the different excitation energy. Raman spectra was measured by using an Argon ion laser with λ =514 nm and λ = 488 nm.

We have established that for the lowers excitation energy (λ = 514 nm) D peak is more intense than the G peak, and its intensity decreases with increasing of excitation energy (λ = 488 nm). Whereas the G peak position is practically independent of excitation energy, the D peak shows a variation of its position. The D mode can not be a simple Raman mode. The two bands G and D representing the same basic Raman active vibration mode of the graphite. The G mode represents the classical zone-centre excitation, the D reports zone-boundary excitations excited via a resonance process, by $\pi - \pi^*$ electron transition. The electron excitation might contribute to Raman spectrum. The excited electron emits a phonon with the same momentum, where the photon absorption took place. There is the resonant Raman scattering with new selection rule.

POTOLUMINESCENCE OF NANODIAMONDS, WHICH INTERACT WITH BIOLOGICAL MOLECULES

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In this work, photoluminescence of nanodiamonds interacting with biological macromolecules, such as proteins, lysozyme and albumin, is studied. Proteins were physically adsorbed on carboxylated nanodiamonds surfaces. The PL spectra of the protein-nanodiamond complex were measured. It is shown that the surface passivation can modify the nanodiamond luminescence band shape.

Nanodiamonds have a strong photoluminescence in the visible range. Protein molecules do not luminescence. However, the adsorption of protein on the nanodiamonds surface changes the luminescence. It is difficult to assume that the lysozyme molecule can greatly change the nanodiamond physical properties at the room temperature.

Our previous measurements showed that the nearest environment of nanoparticles can strongly affect the optical properties of nanoparticles [1,2]. Usually there are graphite clusters on the surface of nanodiamonds, which absorb the exciting radiation and transmit the excitement in nanodiamonds. The presence of protein molecules near the carbon cluster can change the nanodiamond excitation condition because of the interaction of biological molecules and graphite clusters. As a result, the changes of photoluminescence band shape of protein-nanodiamond appear.

This study is important for the bio and medical applications of nanodiamonds used as a biocompatible label.

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[2]. N.N. Melnik, T.N. Zavaritskaya, V.A. Karavanski. "Optical properties of graphite nanoparticles in irradiated diamonds", 2nd conference on New Diamond & Nano Carbons (NDNC 2008), May 26th-29th 2008, Taipei, Taiwan, Abstracts, 260

SPECIFIC OPTICAL PROPERTIES OF NANOCOMPOSITE FILMS BASED ON POLYSILANES RESTRICTED BY POROUS SILICA AND TITANIA

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The organic/nanosize inorganic hybrid materials have a prominent role in the forefront of research due to combining the advantages of organic and inorganic materials and open up countless possibilities for application.

In this work novel composite films based on poly (di-n-hexylsilane) (PDHS) incorporated into SiO_2 [1] and TiO_2 nanoporous films were fabricated. Photoelectronic properties of these composites have been studied using optical spectra and photoluminescence decay measurements in the wide temperature range (5-330) K as well as refractive index of inorganic matrix and composites. It was proved that the polymer chains are localized into the nanopores of inorganic films. These measurements demonstrate essential influence of inorganic matrixes on the polymer chains conformation and the emission properties. It was shown that an intense aggregate photoluminescence is specific feature of newly fabricated composites, and photoluminescence and life time of PDHS/ TiO_2 composites are much lower than that of PDHS/SiO_2 composites, which we attribute to the exciton dissociation at the polymer - TiO_2 interface.

Temperature dependence of photoluminescence intensities enabled us to establish the nature of the conformational structure of the polymer chains as well as to obtain information about the thermochromic transition of the confined PDHS and the excitation energy transfer pathways.

It was shown the strong suppression of nonradiative decay channels and the absence of the thermally activated photoluminescence quenching of embedded nanosize PDHS, what is in contrast to the results obtained for polymer films and solutions. The effect is evidently caused by the reduced exciton migration due to the strong exciton localization in the low-dimensional structure. It is discussed characteristic features of nanocomposite films related to the supervision of intensive photoluminescence even at a room temperature.

[1]. N.I. Ostapenko, N.V. Kozlova , E.K. Frolova et.al., J. Appl. Spectr., 78, 1, (2011) 82.

FUNCTIONALIZATION OF NANO-EXFOLIATED GRAPHITE

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The work is devoted to questions of interrelations between methods of functionalization and functional groups distribution character on the surface of nanographite plates. Functionalization of initial thermoexfoliated graphite (TEG) was carried out with using of inorganic reagents such as $KMnO_4$ solution in the sulfuric acid and mixture of sulfuric and nitric acids and during different time of first and re-dispersion in the magnetic stirrer. Quantitative and qualitative composition of functional groups on the nanographite plates surface was determinated by infrared spectroscopy method.

As it is revealed from detailed studies of structure of the functionalized graphite the fuctionalization results in destruction of initial TEG structure and reduction of TEG particles size under some nanometers (Fig.1). The IR absorption spectrum for functionalized TEG is presented at Fig. 2
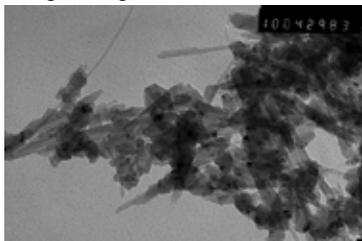
Fig.1. TEM image of nano-exfoliated graphite particles functionalized with $KMnO_4$ solution in sulfur acid.
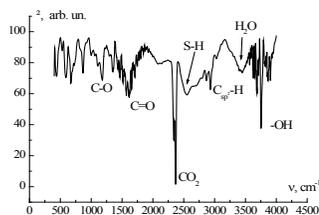
Fig.2. The IR spectrum for nano-exfoliated graphite functionalized with $KMnO_4$ solution in sulfur acid.

As it should be from figure the IR spectrum contains intensive peaks, which correspond to the valence vibrations of the hydroxyl –OH group (3750 cm^{-1}), hydrogen atoms bonded with sp^2- and sp^3- hybridized carbon atoms (3000 cm^{-1}), C=O double bond (1800-1650 cm^{-1}), lactone group (1450 cm^{-1}). The intensity of these peaks in the IR spectra for specimens with bigger repeated dispersing time is weaker.

PECULIARITIES OF MAGNETIC PROPERTIES OF NANOCOMPOSITE $Ba_6Mn_{24}O_{48}$ AT LOW TEMPERATURE

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Static and dynamic magnetic properties of nanostructured compound $Ba_6Mn_{24}O_{48}$ was investigated in temperature range 4.2-100 K in magnetic fields up to 6 kOe. Two types of samples were investigated: a powder and a compacted powder. The magnetic moment temperature dependences M(T) for both samples demonstrate an anomaly around 50 K caused by phase transition in the magnetically ordered state.

Temperature dependences of magnetic moment measured in field cooling (FC) and zero field cooling (ZFC) regimes in magnetic fields from 24 to 3000 Oe are strongly different for two type of samples. Magnetization at 4.2 K in a field 200 Oe differs by almost two-fold. Existence of splitting point between FC and ZFC regimes indicates that in this compound exists a phase separation at low temperature. The temperature of the splitting for both samples, T * is weakly dependent on the external magnetic field. This indicates that the compound is in a state of spin glass.

The study of the temperature dependence of the dynamic magnetization of pressed powder $Ba_6Mn_{24}O_{48}$ in the frequency range 10 - 10 000 Hz allowed to determine the frequency dependence of the freezing temperature T_f. Based on these data determined the rate of frequency shift of the freezing temperature T_f

$$\delta T_f = \frac{\partial \textbf{h}\ T_f}{\partial \log_{10} \omega} \approx 0.013 \quad ,$$

the resulting value is consistent with similar estimates for the spin - glass systems.

SPECTROSCOPIC STUDY OF CATIONIC CARBOCYANINE DYES BINDING TO LIPOSOME VESICLES

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Organic dyes are still widely used in biological researches and medical diagnostics as fluorescent markers and probes for cell and tissue imaging and tracing, studying different processes taking place in living cells. Fluorescence labeling of non-fluorescent nano-scale vehicles such as liposome vesicles, polymeric micelles, latex nanoparticles, polymeric spheres is also powerful tool for studying their fate in living organisms. Organic dyes can be introduced in nano-scale vehicles either by covalent labeling or by adsorption. The latter way can supply researches with additional information concerning the probe environment. However, since electrostatic, hydrophobic and van der Waals forces between the probe and the target can be very specific, it can affect the interpretation of the data obtained in biological research. So, the specificity of probe-to-target interactions could be taken into consideration.

In present study, the interaction of series of hydrophobic cationic carbocyanine dyes 3,3'-dioctadecyloxacarbocyanine perchlorate (DiO), 1,1'-dioctadecyl-3,3,3',3'-tetramethylindocarbocyanine perchlorate (DiI) and 1,1'-dioctadecyl-3,3,3',3'-tetramethylindodicarbocyanine perchlorate (DiD) with egg yolk phosphatidylcholine (PC) has been studied spectrophotometrically in aqueous solutions. Using the modified Scott equation, the binding constant (K_c) of the dye to PC liposomes at four different temperatures (288, 298, 308, 318 K) have been calculated. The thermodynamic parameters (the standard free energy change (ΔG) of the dye transfer from water phase to lipid phase, enthalpy (ΔS) and entropy (ΔH)) of this complex were calculated from the K_c values at different temperatures by the usual method. The calculated K_c values for all dyes are very high that indicates the strong interaction between the dyes and lipid bilayer of liposomes. The increase in temperature causes the decrease in the binding constant for all dyes. It is evident that at higher temperature the tendency to form the dye-to-liposome complexes lessens. The high negative values of ΔG indicate that the process of dye-to-liposome binding is spontaneous and energetically favourable process. Obtained data were used to select tandem dyes for PC liposome labelling in "liposome – cancer cells" interaction studying.

THERMOLUMINESCENCE OF THE NANOCRYSTALLINE ZrO$_2$ – PURE, YTTRIA-STABILIZED AND Cr, Mn, Fe DOPED

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The nanocristalline ZrO$_2$, pure and yttria-stabilized $(ZrO_2)_{1-x}(Y_2O_3)_x$, has been investigated by the thermostimulated luminescence (TSL) method in the temperatures range of *80–400 K* over the composition range *0<x<0.08*. Pure ZrO$_2$ doped with Cr, Mn, Fe was also studied.

The TSL glow curve of pure zirconia, 3.4 mol. % and 8 mol. % YSZ (yttria-stabilized zirconia) is shown in Figure. The TSL glow curve of pure zirconia contains four intensive peaks at *100, 131, 184, 258 K*, at least two of them are complicated. TSL glow curves of YSZ consist of several strongly overlapped peaks in the range of *85-200K*.

The trap activation energy values for 3.4 mol. % YSZ were determined using the fractional glow curve method. The calculated energy values are in the range of *0.15–0.5 eV*. As it occurred the trap activation energies for this specimen can be described by formula $E=\hbar\omega n$, where $\hbar\omega=0.050\ eV$ (*404 cm^{-1}*), n assumes integer values. The corresponding vibration band (*403 cm^{-1}*) was found in Raman spectra of nanocrystalline YSZ. For the sample 8 mol. % YSZ the trap activation energy values change continuously from *0.15 eV* to *0.45 eV*. We consider that it caused by the changes in the thermoluminescence mechanism due to increasing of the impurities concentration.
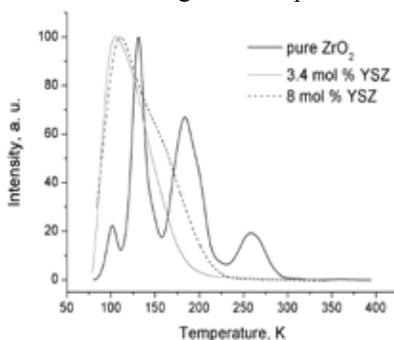
FABRICATION AND OPTICAL PROPERTIES OF FUNCTIONAL OPTICAL ALUMINA AND ZIRCONIA NANOCERAMICS

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The optical absorption spectra, Raman spectra, and photoluminescence spectra of optical oxide nanoceramics ZrO_2 and α-Al_2O_3, obtained under conditions of high 5, 7 GPa pressure using high-pressure apparatus such as Bridgman anvils with toroidal depression and a hydraulic press with the capacity 2000 tons have been studied. Phase composition and crystal structure of the samples have been studied by X-ray analysis. Diffraction patterns of samples were recorded in filtered copper radiation with an automated X-ray diffractometer DRON-3. Optical absorption spectra were recorded with an automated spectral complex on the basis of single monochromator MDR-3 at room temperature in a wide spectral range (370 – 1100 nm). Raman spectra were obtained using automated spectral complex based on double grating spectrometer DFS-24 in the backscattering geometry (λ_{exc} = 514.5 nm). Emission and excitation spectra were obtained at room temperature using a Cary Eclipse fluorescence spectrophotometer (Varian). The obtained absorption spectra of the investigated oxide nanoceramics based on ZrO_2 and Al_2O_3 nanopowders show that these nanoceramic materials are transparent in the visible range (400 to 800 nm). Nevertheless the weak bands at 437, 448, 454, 464, 477, 491, 554, 576, 583 nm have been observed in absorption spectra of zirconia. The absorption spectrum of Al_2O_3 sample demonstrates the clearly observed absorption minimum at 773.5 nm and a weak feature in the area of 340 nm. A characteristic feature of Raman spectra of all samples is the presence of a strong fluorescence background. However, even in the case of small signal to noise ratio in the Raman spectra all the bands characteristic to monoclinic zirconia have been reliably recorded. For Al_2O_3 sample only one weak band at 97 cm^{-1} has been obtained in Raman spectrum. ZrO_2 sample,

obtained under conditions of high pressure (7,5 Gpa), demonstrates not only typical qualitative Raman spectrum but emission spectrum with a maximum of 405 nm and corresponding excitation spectrum with a maximum at 335 nm, that confirms the fact of formation of crystal lattice in this material. Group of bands in the region of 450-600 nm fluorescence spectra can be caused by the presence of oxygen vacancies.

HIGH-RESOLUTION RAMAN SPECTROSCOPY OF PHOTOPOLYMERIZED AND NONPOLYMERIZED FULLERENE FILM IN WIDE TEMPERATURE RANGE

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Fullerene is a promising material for different applications. In spite of the essential number of articles on fullerene, published in literature for last years, some fundamental characteristics have not been studied properly yet. In this report the results of studies of photopolymerized and nonpolymerized fullerene film of high-resolution Raman spectroscopy in wide temperature range were presented.

Polymerized and polymerized partly (up to 45%) fullerene films were obtained under using simultaneous fullerene deposition and irradiation with ultraviolet light [1]. In the low temperature Raman spectra of these films the bands corresponding to chains and dimers of photopolymerized fullerene located at 1461 cm^{-1} and 1466 cm^{-1}, respectively, have distinguishing peaks, in contrast, to earlier Raman spectra of these films obtained with lower spectral resolution at which only one asymmetric band was observed [2] This observation gives an opportunity to characterize different fullerene polymeric phases in detail.

A small upshift (~2 cm^{-1}) of the peak position of the fullerene monomer at 1469 cm^{-1} is revealed at 5 K when the degree of the fullerene film polymerization increased. This shift can be explained by the transformation of the surrounding around monomer molecules because of polymerization.

At temperature increase from 5 K till 290 K peaks position of lines corresponding to monomers, dimers, trimers and chains in photopolymerized films are downshifted by about ~1 cm^{-1}. However, in the nonpolymerized film the peak of line assigned with of $A_g(2)$ mode (1469 cm^{-1}) is upshifted, at first, but upper 250 K this peak is downshifted. It should be noted that the change of the direction of the temperature dependence coincides with the fullerene phase transition

At low temperature for nonpolymerized fullerene film a few additional bands are observed in the region of $A_g(2)$, $H_g(7)$, $H_g(8)$ modes (1400-1600 cm^{-1}), the origin of which is discussed.

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A MECHANICAL ACTION OF LASER LIGHT ONTO THE SUB-MICRON SIZED SOLID PARTICLES

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The ability to manipulate, remote control and move small particles by the radiation pressure is useful tool for manipulation microscopic objects, including solid state micro-, sub micro and nano sized particles, living cells, atoms and molecules. The small particles manipulation by laser tweezers is widely used in a variety of science and technology applications, particularly, in biology and medicine. The ability of laser manipulation of small objects strongly depend on the object size, its optical properties and laser beam parameters. The micron sized transparent objects are rather convenient for such control, in contrary, light absorbing particles needs the special shape of laser beam . Very attractive applications of laser tweezers in nanotechnology need the study of fundamental processes of light mechanical momentum transfer from light to nano-sized particle.

We have developed and studied the optical tweezer for absorbing particles based on the digital holography approach to the shaping of laser beams.

Holographic techniques significantly extend the capabilities of laser tweezing, making possible extended trapping patterns for manipulating large numbers of particles. The methods for creating arbitrary configurations of optical tweezers using computer-generated diffractive optical elements are under the development in many laboratories. We propose the effective algorithms of calculation of phase distribution for phase masks and diffractive elements. The experimental techniques of laser beam control with spatial light phase modulator were tested and studied. The ring-shaped laser beams were generated and used in laser tweezer to manipulate by the absorption particles in solutions.

The possible mechanisms of resonant light pressure on the nano sized particle are discussed and theoretical estimation of light force are presented.

INFLUENCE OF MORPHOLOGY OF THE GOLD NANOCLUSTER ENSEMBLE ON THE SERS OF DYE FILM

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Gold nanoclusters (AuNc) are using for Surface Enhanced Raman Scattering (SERS) spectroscopy of various organic compounds. We developed the method for the production of the AuNc by evaporation and co-deposition of polytetra-fluoroethylene (PTFE) and Au in vacuum. During co-condensation and composite film growth Au forms nanoclusters which size in first instance, dependent on the Au concentration. The AuNc size distribution is about 4-9 nm at Au concentration about 15 %(vol). The mean size of the AuNc can be increased from 7 nm to up to 50 nm with annealing of the as-deposited Au-filled PTFE films to 300^0C. Thin films of the rhodamine 6G and squaraine dyes were deposited by evaporation in vacuum onto substrates with different AuNc morphology. The SERS spectra obtained are in good agreement with the known ones for Rhodamine 6G. The larger AuNc, the higher SERS signal. But the intensity of the Raman signal and signal-to-noise ratio are also dependent on the parameters of the whole AuNc ensemble morphology. The final morphology of the AuNc ensemble dependent on the Au concentration, film thickness and annealing temperature. The AuNc –PTFE system seems very perspective as chemically and biologically inert substrate for SERS spectroscopy of various organic compounds.

THE EFFECTS OF STRONG VIBRATION-ELECTRON INTERACTION IN VIBRATION SPECTROSCOPY OF C_{60} FULLERENES AND LIMITATIONS OF QUANTUM-CHEMICAL CALCULATIONS

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Fullerenes C_{60} and $C_{60}Sn$ are good model objects for the quantum chemical calculations and further comparison with experimental results by methods of vibration spectroscopy. The aim of this work is seek of limitations of quantum mechanics at its application to the complicate objects, in which great role plays nonlinear resonance interaction of vibration bands [1]. The limitations are revealed in phonon discrecity of condensed matter of heat of phase transfer and vibration nonstability of the condensed matter structure [2]. All these phenomenon are caused by strong vibration-electron interaction (VEI), that is not accounted in the quantum chemical interaction and at calculations of normal vibrations. In Raman and IR spectrums strong VEI are revealed in the anomalous amplification of vibration bands, appearance of background and casual wide band that correspond to electron ones [2]. Numerical calculations of geometrical configurations and binding energy, vibration frequencies and activities of all bands in the RS and IR spectrums for the molecules C_{60} and $C_{60}Sn$ are done in Gaussian-03 program with use of Hartree-Fock method.

Differences of calculated and observed vibrations sharply increase with increase of the frequency, achieves up to 200 cm^{-1} and cannot be accounted by scalable multiplier. Discrepancies were revealed for the intensities of theoretical and experimental bands. In C_{60} observed bands Hg(3), Hg(7) are in 4,5 and 6,7 times higher, bands Hg(5), Hg(6) are weaker. That is explained by existence of the frequent resonances Hg(1)+Hg(2)=Hg(3) and 2Hg(3)≈Hg(7) and strong VEI, that is confirmed by observation new electron bands near Hg(3,7) modes with half widths 80 and 150 cm^{-1}. Increase of changes in electron polarizability for Hg(3,7) bands we explain by amplification of delocalization of electron density and its sensivity to vibrations. Redistribution of the trans-

ferred charge 0,977e from Sn to C_{60} in numerical calculations leads to rise of Hg(3,7) bands intensity in 2 times, decrease of Hg(6) in 2 times. This points on necessity of new conception in quantum-chemical calculations.

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6
SURFACE

TRANSLATIONAL DIFFUSION OF COLLOIDAL PARTICLES AT A FLUID INTERFACE

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Colloids at fluid interfaces have attracted much attention in the past years as model systems for fundamental questions as crystallization, melting, gelation.... In front of these extended studies and despite the interest for applications (Pickering emulsions, froth flotation,..) less attention has been paid to the measurement of their dynamical behavior [1-2]. The aim of this contribution is the study of colloidal diffusion at a fluid interface.

Spherical colloids with different surface wetting properties have been studied. Wetting properties are important to address open questions such as the influence of the interfacial confinement on the effective viscosity, the specific coupling between the rotational and translational diffusion, the influence of the morphology induced interface deformation on the particle diffusion,..

In the experiment, colloids of micrometric size are trapped at air/water and air/hexanol interfaces by a spraying technique to avoid surface contaminants. The position of the particle with respect to the interface is finely adjusted via the colloid contact angle. On silica beads this angle can be easily tuned in the range 30°-140° by controlling the surface density of a silane-based hydrophobic agent. A new home made technique coupling Vertical Scan Interferometry and particle tracking allows measuring the diffusion coefficient of the particle as well as its radius, its contact angle and possible interface deformation.

The diffusion of spherical particles at the interface is faster than in the bulk and strictly different from the theoretical models predictions [3]. The difference could be explained taking into account possible couplings between the rotational and translational diffusion and the particle induced surface deformation which were not taken into account in the models.

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IMAGE FORCES FOR DIPOLES NEAR METAL SURFACES

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The method, previously elaborated for calculations of charge image force energy [1] was applied to point dipoles. Theory describing point-dipole image force energy near the surface of the condensed-matter substrate was developed taking into account the dipole screening by free or bound charges in the adjacent medium. The screening is characterized in terms of the dielectric permittivity with spatial dispersion. The dipole orientation with respect to the surface plane is considered arbitrary. It is shown that the classical dependence r^{-3} of the dipole attraction to the surface, where r is the distance between the dipole and the surface, should be drastically modified by the substrate. Specific calculations were carried out for metallic substrates in the Thomas-Fermi and Schulze-Unger-like approximations for the dielectric permittivity. The latter makes allowance for the quantum-mechanical character of screening at small distances (large transferred wave vectors).We found that in the case of the quantum-mechanical screening the image-force energy of the horizontally oriented dipole diverges as r^{-1}, while that for the normally oriented dipole is finite at $r \to 0$. In the classical theory, dealing with the ideal conductor, which possesses the infinite dielectric constant, the dipole orientation perpendicular to the surface is always energetically favorable. On the contrary, we have shown that this orientation is preferable only at long r, whereas near the surface dipoles should be directed along the surface. Our findings demonstrate that any results in the theory of adsorption obtained in the framework of the classical electrostatic approach should be regarded with caution .

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TWO-LAYER POLARITON ELLIPSOMETRIC SENSORS FOR SMALL MOLECULAR CONTAMINATION ON THE BASIS OF THIN TRANSITIONAL METAL AND GOLD FILMS

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Single-layer sensors for small molecular contamination based on polariton measurements are made on the basis of thin translucent gold films, evaporated on hypotenuse edge of the prism of the total internal reflection or on central cut semi-cylinder from glass or quartz. But gold films have weak adhesion to glass or quartz, therefore such sensors have a short life-time. In the same time it is known that transitional metals, on the contrary, have high adhesion to glass and quartz. So we have calculated the sensitivity of the row of polariton ellipsometric sensors made on the basis of two-layer thin films Ti-Au, Cr-Au, Ni-Au and Mo-Au. Such sensors must be charaterized by a mush longer life-time, than single-layer on the basis only gold films. The calculated sensors work as ellipsometric sensors with change the angle of incidence under constant length wave. The calculations of such sensors with excitement of surface polaritons were organized on base of recurrence Airy formulas for three-layer thin film system. The index of refraction of the glass prism was 1,52. The length of the light wave $\lambda = 620$ nm. The indexes of refraction and absorptions for gold and above mentioned transitional metals were taken from reference book. Excitement of surface polaritons by Krechman method was considered. Ellipsometric parameters tgΨ and cosΔ (Ψ-azimuth of restored linear polarization, Δ- phase shift between p- and s-component of the reflected wave) were calculated, since exactly these parameters are measured ellipsometric Beatty method. First, tgΨ and cosΔ for clean unpolluted surface of the sensor were calculated, then for surface on which a thin film of the lavender butter with index of the refraction 1,46 was inflicted. Was defined such thickness of the film of the lavender butter, under which difference of the values tgΨ and cosΔ for clean surface of sensor and surface with film of the lavender butter, still exceeded absolute accuracy of the measurements. The received results have shown that more sensitive is parameter cosΔ. Exactly by latter the thickness of lavender butter film was defined. So for sensor Ti-Au and Ni-Au this thickness turned out to be 1Å. For sensor on base of Cr-Au and Mo-Au films - 5Å. Thereby it is necessary to note that sensors on base of two-layer film Ti-Au and Ni-Au allow confidently determine monoatomic superficial layer of polluting material. The most sensitive angels of incident of the light on sensor were also determined. They turned out to be: Ti-Au -44^0, Cr-Au-64^0, Ni-Au-44^0 and Mo-Au-58^0.

PROPERTIES OF WALL-ADJACENT ELC LAYERS

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Surface forces field of the solid substrate induces in wall-adjacent layers of some liquids orientationally-ordered qusy-phase similar to nematic phase and called epitropic liquid crystalline state (ELC). This state is separated from the bulk isotropic liquid by relatively sharp boundary. The ELC thickness depends on the substrate nature (dielectric or conductive) and varies from hundreds to thousands of molecular lengths, the order parameter of ELC layers is about 0.2-0.3.
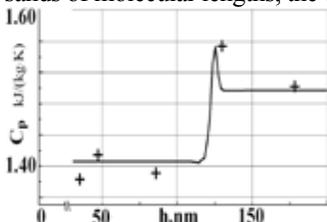
Fig.1
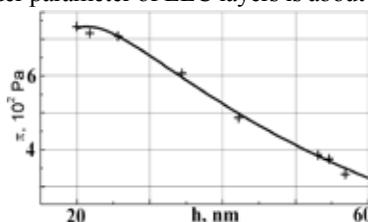
Fig.2
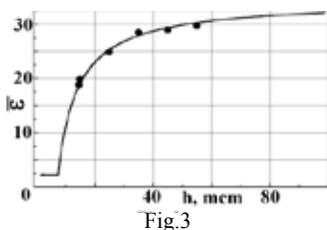
Fig.3

We tried to fulfill a theoretical interpretation of previous experiments of different physical characteristics of ELC layers – thickness dependencies of heat capacity (fig.1), disjoining pressure (fig.2) and mean value of dielectric permittivity (fig.3). Studied liquid was nitrobenzene bounded by quartя (1,2) and steel (3) substrates. Calculations were done in the framework of early proposed model of ELC spectral properties [1], which take into account dipole-dipole and disperse interaction between liquid particles and disperse interaction between these particles and solid substrate.

Fig 1 illustrates the evidence of jump in   behavior, which is conditioned by the transition from ELC to isotropic phase. Fig.2 illustrates 2 zones of dependence: in the range h<25 nm molecular part prevails and in case of h>25 nm – structural part of disjoining pressure prevails. Fig. 3 illustrates peculiarities in dependence of symmetrically bounded interlayers. It is explained as the manifestation of two-component nature of ELC layers – sandwich-type dimers (with compensated dipole moments) dominate in wall-adjacent ELC layers and their evidence lead to decreasing of dielectric permittivity.

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REFLECTION/TRANSMISSION SPECTROSCOPY FOR METAL NANOPARTICLE/NANOWIRE ARRAYS ON THE SEMICONDUCTOR SURFACE

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Spectroscopy of transmission enhancement into semiconductor substrate through a nanostructured conductive (e.g. metal) layer has applications in photovoltaics, sensors and various non-linear optoelectronic devices (see e.g. [1]). However, for experimental study of these phenomena, the reflectance spectroscopy is more preferable. Therefore in this report the theoretical analysis and numerical calculations of light transmittance/reflectance for ensembles of metal plasmonic nanoparticle/nanowire arrays with excitation of local (surface) plasmons (SP) and surface plasmon polaritons (SPP) has been performed.

Using curvilinear coordinate transformation method [2], the spectra of reflectance/transmittance were calculated for s- and p- polarized light incident on the periodic system of Au nanoparticles/nanowires on the GaAs substrate. First of all, the obtained spectra contain peculiarities corresponding to the diffraction orders of SPP excitation. In the same time, these spectra have very smooth form for averaged flat gold films with the identical mass thickness. Besides there are other peculiarities due to excitation of local (SP) plasmons in nanoparticles or on the cross-section of nanowires. The transformation of local plasmons into SPP with the filling factor (by metal) increase is predicted. Analysis of the spectral peculiarities of reflectance/transmittance indicates the asymmetric Fano resonance shape as a characteristic feature of interacting quantum systems [3]. In our case, apparently, the light excited SPs across the metal nanowires (nanoparticles) interfere with SPP's of the 1D (2D) their array. Namely, the Fano lineshape is usually conditioned by interaction of narrow discrete resonance (e.g. Frohlich local mode SP) with a broad spectral line of continuum (e.g. SPP diffraction modes). As unique asymmetric shape of Fano line for plasmonic systems as the effect of transmittance enhancement in the conductive layers on semiconductor substrate are discussed in this report as applied to polaritonic sensors and plasmonic solar cells.

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VIBRATIONAL SPECTROSCOPY OF AMORPHOUS ICE

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Investigation of amorphous ice has attracted considerable attention because of its importance for atmospheric sciences, environmental studies as well as for broad practical applications in cryobiology and astrophysics. In this work the results on FTIR spectroscopic study of dispersed amorphous water ice, adsorption and reactions of some molecules on its surface are presented.

The cryostat cell for spectral studies of adsorbed molecules at variable temperatures (55-370 K) and the device for water film deposition were described elsewhere [1].

The estimated specific surface area of freshly deposited at 77 K water ice film is about 160 m^2/g and decreases on raising the temperature together with intensity diminution of the bands due to the dangling OH (OD) groups at 3696 (2727) cm^{-1} until the disappearance of the latter at 130 – 160 K when the changes of bulk absorption of ice provide evidence for the transition from amorphous to polycrystalline phase [1]. CO adsorption at 77 K results in two bands at 2153 and 2137 cm^{-1} assigned to molecules forming weak H-bond with the dangling hydroxyl groups or bound to unsaturated surface oxygen atoms, respectively. Adsorption of different molecules results in the low-frequency shifts of the band of dangling OH groups [2]. Besides, spectra of adsorbed N_2, CO and CH_4 registered at 55 K reveal absorption intensity decrease at ~ 2650 cm^{-1} at the high-frequency side of the bulk absorption, and increase at about 2625 cm^{-1}. This new effect we interpret as a result of strengthening of H-bonds between surface water molecules, which act as adsorption sites either as proton-donors or as donors of the lone pair of electrons.

Surface of ice particles plays the role of a condenser of atmospheric pollutants and acts as a micro-photoreactor in the atmosphere. This is illustrated by the results on study of such ecologically important reactions like ozone photolysis and ozonolysis of chlorinated ethenes and hydrogen cyanide at 77 – 200 K.

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PHOTODEGRADATION OF ADSORBED DYES ON THE SURFACE OF MESOPOROUS SIO$_2$, TIO$_2$ AND SIO$_2$/TIO$_2$ FILMS

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A detailed knowledge of the photostability and photodecomposition of dyes when adsorbed on the oxide surfaces in air is desirable to monitor the transition products of the destruction. The aim of the work was to investigate the effect of photocatalytic porous TiO_2, TiO_2/SiO_2 and SiO_2 film surfaces and photoinduced superhydrophylicity of TiO_2 films on the mechanism of dye photobleaching under UV irradiation by combination of UV-vis spectroscopy and laser desorption/ionisation time-of-flight mass spectrometry. We synthesized the mesoporous TiO_2, TiO_2/SiO_2 and SiO_2 films, tested these films as wafers for Laser desorption/ionisation (LDI) mass-spectrometry and *in situ* studied the kinetics of adsorbed thyazine dye Methylene Blue (MB) and acridine dyes Acridine Orange (AO) and Acridine Yellow (AY) photobleaching.

The transparent porous thin films were synthesized via low-temperature sol-gel route in presence of template agents having the developed porosity and the high surface area. The developed porous structure is favorable geometrically for an entrance of two and more dye molecules. The associates of MB, AO and AY in porous silica gel are formed beginning with the covering ~0.01% of monolayer when the ratio of Dye:OH groups is app. ~1: 600. On the surface of mixed TiO_2/SiO_2 the adsorption of organic dyes is remarkably increased due to the enhancement of surface acidity and surface hydroxylation.

Metachromasy effect (the dye aggregation followed by change of color with a hypsochromic spectral shift due to repulsive interactions, which induce shifts to higher energies) coincide with photoinduced superhydrophylicity of TiO_2 films.

Photodegradation of adsorbed MB, AO and AY on the surface of researched films in air leads to the formation of various transient intermediates depending on the film composition. In presence of titania, photobleach of adsorbed dyes occurred faster in comparison with this process in presence of pure silica. We suggest that formation of active oxidative species like singlet oxygen and/or hydroxyl radical under UV irradiation of adsorbed dye molecules leads to the full degradation and discoloration of adsorbed dye. Efficient photodegradation of MB, AO and AY occurs through following steps: 1-N-demethylation (deamination for AY); 2-photodimerization; 3-photodegradation.

VARIABLE-TEMPERATURE IR SPECTROSCOPY FOR STUDYING THE THERMODYNAMICS OF REVERSIBLE GAS-SOLID INTERACTIONS

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Reversible gas adsorption on porous solids constitutes the basis of a wide range of technological processes; among them, gas separation and purification (based on selective gas adsorption), gas sensing, and gas storage and transport. Variable-temperature infrared (VTIR) spectroscopy was shown [1-2] to be a very sensitive technique that has the potential to discriminate between different adsorption site types that can be present in the adsorbent and, simultaneously, to give precise values of the corresponding (site specific) adsorption enthalpy and entropy that rule the thermodynamics of the gas adsorption process. In addition, knowledge of the characteristic IR absorption bands of the adsorption complex helps to correlate structure and function of the porous adsorbent.

The basis of the VTIR method will be highlighted, followed by a perspective of recent developments, combining VTIR spectroscopy with periodic DFT calculations [3], relevant to the fields of hydrogen storage [4-5] and carbon dioxide capture and sequestration (CCS) [6-7]; which bear high interest in the context of present day issues related to energy and environmental science.

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INFRARED SPECTROSCOPY OF SURFACE SPECIES

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The lecture deals with the advances in the IR spectroscopy of adsorbed molecules and surface species. Vibrational spectra of surface compounds provide unique information about the structure of adsorbed layers, properties of surface sites, about the effect of strong surface electrostatic fields upon the molecules and the nature of intermolecular interactions. They are not complicated by the rotational structure and can be studied in a broad range of temperatures, not limited by points of condensation or crystallization as in solutions or matrices.

Cell technique for spectral measurements at variable temperatures is considered, as well as the methods of studying the samples of different nature, such as oxides, metals, salts, films of porous ice. The influence of scattering upon the spectra of pressed powder samples is analyzed. Special attention is paid to the application of isotopic substitution for the establishing the structure of surface species.

The advances of FTIR spectroscopy for the studies of surfaces are illustrated by the examples of weak surface complexes of simple molecules. Spectral manifestations of H-bond, both conventional as well as the blue-shifting are discussed.

The mechanism of lateral interactions between the adsorbed molecules on oxides includes strong repulsion caused by the static effect, whose mechanism includes relaxation induced by adsorption, and the dynamic coupling, that shifts the bands and affects their shapes. Co-adsorption of acid and basic molecules demonstrates the effect of induced acidity or basicity, when the strength of surface sites changes dramatically due to the presence of weakly adsorbed molecules.

Recently it was shown that CO reveals linkage isomerism and forms with surface cations both C-bonded and O-bonded complexes, which coexist in thermodynamic equilibrium. Surface isomeric states were established for some other adsorbed species, such as cyanide ion CN^- produced by HCN dissociation. The existence of linkage isomerism can be explained by a simple electrostatic model, which also predicts a correlation between the frequency shifts on adsorption and the integrated absorption coefficients. The experimental results are in a fair agreement with the theory.

SPECTROSCOPIC PROPERTIES OF ORGANO-MODIFIED MONTMORILLONITES. EFFECTS OF MULTIWALL CARBON NANOTUBES DOPING

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The structure and photoluminescent properties of natural montmorillonite (MMT) aluminosilicates from three mineral deposits (Askan, Cherkassy and Pyzhevsk), which differed in the inorganic impurity contents and cation-exchange capacities, and were modified by cations of sodium or the surfactant cetyltrimethylammonium bromide (CTAB) have been investigated. Photoluminescence emission for these materials can be reached only at helium temperatures and does not appear at room one. X-ray fluorescence analysis showed significant differences in the concentrations of the inorganic dopants in these materials. An X-ray diffraction analysis established that incorporation of the CTA^+ long-chain cations into the MMTs expands remarkably the mineral interplanar distances, the values of which are close to each other for all organoclay samples under study and equal to 1.8–2.0 nm. The photoluminescent properties of the Na-form of the MMTs are shown to depend on the amount of introduced dopant capable of either enhancing or quenching the emission. Deposition of CTAB on the mineral surface influences the luminescence pattern, the spectral contour and wavelength range being practically the same for all modified samples. The emission may intensify or weaken because of such surface modification.

A method to modify a montmorillonite (MMT) clay mineral surface by surfactant cations with simultaneous doping by multiwall carbon nanotubes (MWNT) has been proposed. Samples with MWNT do not luminescence at all, since the MWNT contain traces of contaminating iron cations, which probably, quench the emission. Studies of these composite materials by IR-spectroscopy have revealed the mutual influence of the components appearing as the ordering of near-surface layers in the aluminosilicate framework and a change in the modifier methylene chain con-

formation at the interphase boundary. The majority of CTAB (~90%) is shown to be located inside the MMT galleries, the packing arrangement of which depends on the cation-exchange capacity value and affects the interplanar distances in MMT. The alkyl chains of the CTA^+ cations on the outer surface of the MMT plates are sorbed by nanotubes, thus providing contact between the organoclay and MWNT surfaces.

EFFECT OF SOLVENT ON OPTICAL TRANSMITTANCE OF POLYMER CARBON SUSPENSIONS UNDER POWERFUL PULSED LASER EXCITATION

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The kinetics of transmittance was investigated using a pump-probe scheme in the suspensions of carbon microparticles in liquid polymer (epoxy resin without addition of a hardener) with small amount of the solvent (acetone) adding. For suspensions preparation the method of laser ablation was employed. As a result, epoxy carbon suspensions with the average particle diameter of about 130 nm and with approximate particles concentration of $0.2*10^{10}$ cm^{-3} were obtained. The investigated suspension was exposed to irradiation by a single laser pulse (YAG:Nd^{3+}, pulse energy 20 mJ).

The basic physical effect at the laser irradiation of light-absorbing microparticles both in gases and in condensed matter is their heating up to high temperatures of approximately 4000 K. Such particle heating in polymer matrix is accompanied by laser-induced incandescence (LII), which is clearly visible, and by the phenomenon of optical limiting (OL), due to the self-action of laser irradiation in the sample.

In the transmittance kinetics the main mechanism of optical transmittance decrease is laser-induced scattering, which involves Mie scattering by microbubbles formed in the vicinity of overheated carbon microparticles and filled with gaseous products of pyrolysis of epoxy resin. After a small amount of solvent adding to the polymer suspension, the kinetics of transmittance changes significantly. Changes in the solvent concentration lead to significant changes in the transmittance kinetics, which can be used as a tool for detection of solvent presence in the polymer.

MEASUREMENT OF DEPOLARIZATION OF LIGHT SCATTERED FROM DIELECTRIC STRONGLY SCATTERING SAMPLE

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Industrial usage of noncontact methods for measuring objects parameters and material they consist of currently is sufficiently large. Goniophotometric measurement is one of these methods. Depending on the type of substance, from its scattering abilities one can gain its purity, surface structure, statistical distribution of its particles or other relevant information, according to properties which influence on substance scattering abilities.

In this work we studied scattering properties of dielectric samples made of standard glass MS-20. For the measurements we used goniophotometric device based on goniometer G-5. Sample was illuminated with s and p linearly polarized light. At the same time, we observed scattered light through linear polarizer to obtain s and p polarization component of scattered light. Thus we could analyze depolarization of light after scattering. During the experiment we gained luminance of scattered light with respect to luminance of propagation light, for the illumination angle 0, 45 and 60 degrees, and four combination of polarizer and analyzer state. Gained data correspond to behaviour of strongly scattering low-absorbing samples.

LASER-INDUCED INCANDESCENCE OF CARBON SURFACE

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Laser-induced incandescence (LII) is a well-known type of laser-induced emission observed in light-absorbing microparticles under powerful pulsed laser irradiation. LII is easily observed in suspensions and aerosols with the use of moderate-power lasers generating nanosecond-timescale lasers. To a naked eye, LII looks like a broadband luminescence.

As a kind of thermal emission, powered by a nanosecond laser pulse, LII possesses properties of nonlinear emission. The intensity of LII, I, at a fixed wavelength nonlinearly depends on the intensity of laser excitation, F, which can be approximated as power function $I = \text{Const} \times F^{\gamma}$ for moderate deviations of F. In carbon suspensions, typically, the factor of nonlinearity $\gamma = 2\ldots5$.

Computer simulations demonstrate that bulk light-absorbing materials can demonstrate LII when irradiated by a nanosecond laser pulse. If the length of thermal diffusion during the laser pulse and the penetration depth of laser radiation are short enough, the surface layer can be overheated to the temperatures suitable for observation of incandescence in the visible spectral range at laser power density of the order of $10\ldots100$ MW/cm^2.

For bulk carbon samples, the experiments confirm the conclusions of the computer simulation. We observed LII with the nonlinearity factor of $\gamma = 7\ldots13$, which is in good agreement with the calculated values. Besides, partial fading of LII is observed with the increase of dose of laser irradiation, which can be attributed to the laser-induced changes of the relief of carbon surface.

It is expected that LII of surfaces of light-absorbing materials can be of use for monitoring of surface parameters and condition.

HIGH REFLECTION EFFICIENCY FOR SURFACE PLASMON RESONANCE BY USE OF METAL-DIELECTRIC FILMS

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Surface plasmon resonance (SPR) is an important property of metal nanostructures, and has been used in application such as optical sensing of biomolecules, photothermal therapy, spectral signal enhancement, photovoltaics [1]. The SPR features of metal nanostructure are highly sensitive to the composition, size and morphology. For gold and silver, the synthesis of nanostructures with controlled size and morphology has led to the production of nanostructures with well-defined SPR absorption features that can be systematically tuned from the visible to the near-infrared spectral range. In case of excitation SPR the intensity of the *p*-polarized light reflected from the glass-metal-air interfaces dropped sharply at some particular value of incidence angle. This reflectivity minimum occurs because surface plasma oscillations absorb the light wave energy at the metal-air interface. The resonant character of the process makes the reflectivity minimum very sensitive to the optical properties of the metal and its environments.

Here, we reported on the excitation of the SPR in Glass/Au/HfO$_2$ multilayer structures. It was found that the reflection efficiency for SPR is dependent on the thickness of dielectric (HfO$_2$) and noble-metal (Au) films. We have analyzed surface plasmon efficiently using of multiple interference effect on the lossy dielectric layer and thin gold film. Our calculations are confirmed by measuring the polarized reflectivity. The standard thin films optics approach, based on the Fresnel coefficients, was employed in order to predict the SPR in the visible spectral range. The reflection and transmission spectra were simulated for an attenuated total reflection setup, also known as the Kretschmann configuration. To be in accord with future experiments, the dielectric functions of the metal and dielectric media are those of the materials deposited in our laboratory. The spectral dependences of the complex refractive index $n + ik = \sqrt{\varepsilon(\omega)}$ for gold film, which used in our calculation, is obtained by a model fitting of the experimental data using two Lorentz functions with a Drude term. The optical constants of the HfO$_2$ film has been parameterized by the Cauchy function with an extinction coeffi-

cient equals to zero. The refractive index of dielectric shows low dispersion with values of n_d=2.04±0.05 throughout the visible and near IR spectral range. Main goal of this calculation is to minimize the *p*-polarized reflection spectra and its half width on the half of high.

At first step the simulation and measurement were done for pure gold film. The thickness 47 nm of gold was obtained by using the Fresnel equations and confirmed by measurement at angle of incidence about 47 deg for wavelength 630 nm. For this thickness the reflectivity minimum is 2-3 % in the Kretschmann geometry. The HfO_2 film on top of Au layer changes the electromagnetic field distribution of the surface plasma oscillation: with increasing thickness of HfO_2, *h,* the field strength at the Au surface increases as well as that part of the energy of the SPR which is transported in the absorbing Au film. A small metal thickness of gold layer can provide the strong coupling the SP to incident waves and excite the SP with sufficient amplitude. Usually metal thickness (40-50 nm for Au) results in very large radiative losses of leakage surface plasmon wave, which does not allow getting large reflection efficiency due to large radiative losses. If we add the HfO_2 dielectric layer with thickness 40-50 nm it is possible to get phase differences between ray reflected from HfO_2 and from glass-gold interfaces equals to 180^0. Angle of incidence (60-70°) should also be appropriate to get phase matching between plasmon wave and incident wave. In this case we have fast leakage surface plasmon wave propagating in complex structure of Glass/Au/HfO_2 layers with relatively small radiadive and dissipative losses (since large amount of wave energy is propagating in lossless HfO_2, and due to existence of negative interference). Due to relatively a small losses and a good coupling to free wave it should have significant influence on reflected coefficient. As result a large part of the incident wave energy will transform into SP waves which causes a small reflection coefficient. Our experimental measurements showed that the reflectivity spectra of the samples with increasing of HfO_2 thickness from 10 to 50 nm for fixing Au (30nm) reach the minimum at plasmonic resonances. Note that the pronounced minimum of reflectivity for *p*-polarized incident light is observed at the photon energies 1.5-2 eV. Half width on the half high of the SPR has smaller values about of ΔE~0.01 eV for structure Glass/Au/HfO_2 than for pure Au (47.5 nm) film (ΔE~0.05 eV). The results presented here were obtained by numerical simulations and experimental measurements and they shows an algorithm for optimization the thickness of metallic and dielectric layers which the surface plasmon propagating makes possible with high efficiency.

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SPECTROELLIPSOMETRY OF AMORPHOUS METALLIC RIBBONS OF $FE_{80}TM_5B_{15}$ (TM=TI, V, CR) ALLOYS IN THE INFRARED

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Optical properties of metals and amorphous metallic alloys in the infrared are connected with intraband electronic transitions [1]. Studying interaction between electromagnetic wave and a surface of a metallic material due to the reflected beam ones carry up some information on the electronic characteristics and atomic structure. The aim of this work is to establish the significance of the substitution of small concentration of one transition metal to another in the $Fe_{80}TM_5B_{15}$ metallic amorphous alloys and its influence on optical properties. Dielectric functions of amorphous metallic alloys of $Fe_{80}TM_5B_{15}$ (TM=Ti, V, Cr) were obtained in the far and the middle infrared (0.05-0.6 eV) via spectral ellipsometry method. Such electronic parameters as a relaxation and plasma frequencies were calculated. The obtained parameters indicate much higher concentration of charge carriers near the Fermi level in the case of TM=Ti, Cr substitution than TM=V one and simultaneously smaller free length path for them. Moreover, these parameters of electronic system are closed enough one to another in the case of TM=Ti and TM=Cr. The results of an analysis of specrtroellipsometric data have established that in amorphous metallic alloys of the abovementioned type at the condition of substitution of Fe atoms by atoms of such 3d -metals as Ti, V, Cr the Fermi level became more closed to a mobility edge of the density of electronic states (at certain concentration of Fe atoms such level may occur into pseudogap). The analysis of dielectric functions of the investigated samples with TM=Cr, Ti makes us sure that in the observed optical phenomena there are only single type of charge carrier. In contrast to these alloys in a case of a sample with TM=V probably there are two groups of charge carriers having different concentration and mobility.

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ELLIPSOMETRIC INVESTIGATIONS OF THE FILMS ON CD- AND TE-SURFACES OF CDTE(111) SINGLE CRYSTALS

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In view of wide application of CdTe in optoelectronics, it is essential to monitor the structure and state of the crystal surface before and after surface processing. The films formed on the CdTe(111) polar surfaces (Cd- and Te-terminated) as a result of storage or different treatments of samples differ in theirs chemical composition, structure and properties. In this work, it was found that the surfaces have different optical constants and thickness. The samples were being stored under ambient air conditions for different time periods. Also chemically etched CdTe samples were studied. The morphology and structure of the surface region of the crystals were monitored by atomic force microscopy and reflection of high-energy electron diffraction. The ellipsometric measurements were carried out in the spectral range of 400-632 nm. The obtained values of the ellipsometric parameters were interpreted using the model of a homogeneous absorbing layer located on an absorbing substrate. The refraction n and absorption k indices of the modified surface layer were calculated on the base of the fundamental ellipsometric equation. The values of n, k and thickness d of the surface layer were obtained for the both surfaces of each investigated sample.

It was found that the films formed on different surfaces of CdTe(111) crystals had different optical constants and thickness. In particular, the refractive and absorption indices of the film on the Cd-terminated side were about 2.6 and 0.43, respectively. The corresponding values for the Te-terminated side were $n = 2.7$ and $k = 0.33$. The thickness of the modified film on the Cd-surface ($d = 10$-18 nm) was a little larger than that of the Te-surface ($d = 9$-16 nm). The films formed on different surfaces of the CdTe(111) crystals after chemical etching were transparent for the used light and had the same optical characteristics ($n = 2.42$) and thickness varying from 1 nm (freshly etched samples) to 10 nm (samples after storage in air for several weeks). The difference in the optical properties of the films on the Cd- and Te-surfaces is due to their different capacities to absorb extraneous elements and oxidize under storage in ambient air conditions for a long time.

APPLICATION OF ISOTOPIC SUBSTITUTION FOR ESTABLISHING THE STRUCTURE OF SURFACE COMPOUNDS

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Isotopic substitution is very helpful when the structure of surface species cannot be unequivocally established from the IR spectrum, as it was for the surface complexes of adsorbed CO [1] or ozone [2]. In this work we used this method to the systems with linkage isomerism, when the suggested structure was based on temperature dependence of band intensities. So, for CO adsorbed on zeolites [3] two bands of stretching vibrations were attributed to C- and O-bonded species (structures 1 and 2 in the scheme). For adsorbed HCN two isomeric forms can be suggested both for coordinately bound molecules (structures 3 and 4) and for CN$^-$ ions arising as a result of HCN dissociation (structures 5 and 6). The aim of this work was to use the data on H-D, ^{13}C and ^{15}N substitution for the assignment of the bands of CO adsorbed on some zeolites and those of HCN on Al_2O_3 and TiO_2
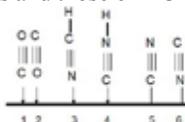
The performed calculation has shown that for adsorbed diatomics the isotopic shift differs from that one, which follows from the reduced mass ratio, and depends on the way of coordination. For C-bonded CO or CN species the shift caused by ^{13}C substitution should be greater than for O- or N- bonded compounds. The difference grows with the increase of the force constant of the bond with the surface. In fact, for the high frequency bands of strongly adsorbed CO molecules on ZnZSM-5 (2233.5 cm^{-1}) and CaY (2186 cm^{-1}) zeolites the shift is 1.0-1.8 cm^{-1} greater, while for the O-bonded species on CaY it is 0.6-1.5 cm^{-1} less, than anticipated from the reduced masses.

To distinguish the bands of molecular and dissociatively adsorbed HCN, spectra of DCN on alumina and titania were studied. The shifts caused by ^{13}C and ^{15}N substitution have shown that molecular adsorption is always as in the structure 3 for both the oxides, while the band at 2190 cm^{-1} of HCN on alumina is due to the N-bonded ions (structure 6), in accordance with the earlier assignment [4].

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VIBRATIONS OF CO ADSORBED ON MOLYBDENUM SURFACES: A DFT STUDY

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Surface vibrational studies using infrared reflection absorption spectroscopy (IRAS) and electron energy-loss spectroscopy (EELS) for CO adsorbed on the Mo(112) and Mo(110) surfaces revealed an unusually low C-O stretching frequency (1130 cm^{-1} for CO/Mo(110)). A disappearance of this mode on heating to 250 K was suggested to indicate this state as a precursor to CO dissociation. Present DFT calculations show that the C-O stretching frequency decreases due to forming C-Mo bonds, which result in the weakening of the C-O bonds. In particular, due to the overlap of the Mo and π-derived CO states,[24] the tilting results in an increase of the C–O bondlength (from 1.13 to 1.17 Å), and, consequently, the C–O stretching vibrational frequency decreases dramatically. In contrast, for CO molecules adsorbed on oxygen-modified Mo(110), as well as for CO molecules forming the second monolayer on the surface, the CO stretching frequency approaches the value characteristic of a free CO molecule. Performed calculations confirm that on Mo(112) and (110) surfaces CO adsorbs without dissociation.

A DENSITY FUNCTIONAL THEORY STUDY OF THE ELECTRON-PHONON COUPLING AT THE AU/MO(112) SURFACE

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Recent advance in high resolution angle resolved photoelectron spectroscopy (HRUPS) allows not only for a direct visualization of the surface electronic band structure, but also for investigations of the subtle details, including the shape and width of the bands in the vicinity of the Fermi level. In particular, the linewidth of the surface bands is originated from electron-electron (*e-e*), electron-phonon (*e-p*), and electron-impurity scattering, which makes the HRUPS, combined with first-principles calculations of the real and imaginary parts of the self energy, one of the major tools for investigation of *e-p* coupling at metal surfaces. The present contribution shows an example of the interplay between results obtained in HRUPS investigations of a clean and (1×1)Au covered Mo(112) surface, and performed DFT calculations of surface electronic bands, phonon bands, Eliashberg functions, and self energy. We have found significant contributions from the surface phonon modes to the low-frequency part of the phonon density of states and Eliashberg function, which result in the enhanced *e-p* coupling at the surface and, consequently, also to an increase of the mass enhancement factor and the imaginary part of the self energy. The DFT calculations indicate that gold overlayers increase the line width of the Mo(112) surface band, crossing the Fermi level at 0.54 Å^{-1}, due to increasing imaginary part of the self energy.

X-RAY PHOTOELECTRON SPECTROSCOPY OF POLYIMIDE SURFACE TREATED BY PLASMA BEAM

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The present study is focused on the XPS characterization of the changes at a polyimide (PI) films caused by an oblique plasma beam treatment, which is presently used as an effective process for LC alignment. The studied samples were the films of PI 2555 from Dupont treated by the beam of accelerated plasma of Ar, Ar/H_2 or H_2 gases generated by the linear anode layer source. The incidence angle of the beam on the PI films was about 70° and the exposure time was 3 min.

The XPS measurements were carried out by using Kratos Axis Ultra X-ray photoelectron spectrometer with a monochromatic Al Ka source operating at 300 W. Survey and high-resolution spectra were acquired at pass energies of 80 and 20 eV and step size of 1 and 0.1 eV, respectively. The survey spectrum was used to estimate elemental content of the surface layer of the film, while the high resolution band C 1s was analyzed to clarify chemical state of carbon atoms in the layer. In the acquisition of all spectra take-off angles q of 90, 60 and 20° were utilized. They corresponded to ~10, ~8, ~3 nm of the sampling depth. To elucidate the in-plane anisotropy of the treated surfaces, the spectra were also measured for the in-plane projection of plasma beam parallel and perpendicular to the incidence plane of testing X ray beam at constant value of take-off angle.

The following results have been obtained. (1) Surface elemental content of the PI samples changes at the plasma beam treatment. The increasing of carbon concentration and decreasing of nitrogen and oxygen concentrations is detected in case of Ar plasma beam. Adding of hydrogen to the working gas enhances substantially this trend. The changes are most severe in the top layer of the film. (2) The best targets for accelerated particles are aromatic and imide rings. In parallel with destruction of these elements, growth of the fraction of hydrogenated carbon is detected. H_2 plasma causes the largest formation of hydrocarbon types of species. The highest concentration of hydrocarbons is detected at the shallower depths that implies that C:H layer is formed on the PI surface. It is seemingly formed from the fragments of destructed polyimide rings. (3) The in-plane anisotropy of treated films is detected, which suggests angularly selective modification of PI surface. The polyimide fragments are stronger destroyed and the hydrocarbon structure is most intensively formed in the direction corresponding to the in-plane projection of plasma beam.

7
BIOMOLECULES AND POLYMERS

DISCOVERY OF HIGHLY EFFICIENT INTRINSIC PHOSPHORESCENCE FROM A SIGMA-CONJUGATED POLYSILANE: NEW CONCEPT OF STRONG ENHANCEMENT OF ISC RATE IN CONJUGATED POLYMERS

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The interest to phosphorescence (Ph) phenomena in organic semiconducting materials has greatly increased in last decade due to creation of highly efficient phosphorescent OLEDs with internal quantum efficiency closer to 100% which was achieved by using organometalic complexes as dopants in such organic matrixes. The reported intrinsic Ph quantum yield for conventional conjugated polymers is usually as small as 10^{-5} or not detectable at all. The combination of a low intersystem crossing (ISC) rate implying a low population of the triplet state, a low radiative rate and a high non-radiative decay results in an extremely low Ph yield for conjugated polymers devoid of heavy atoms.

In this study we report on a highly efficient intrinsic Ph found in a neat σ-conjugated polysilane polymer containing an extended π-conjugated side groups featuring quantum yield as large as ~10% in solid films and 20% in a diluted frozen solution, that is unusually large as for conjugated polymers devoid of heavy atoms and is comparable to that of organometallic polymers. The Ph and delayed fluorescence (DF) in this polymer were studied by time-resolved PL techniques and it was shown that Ph is due to the radiative decay of triplets on side group under excitation of the σ-conjugated polymer backbone, i.e., with energy well below then the lowest singlet state of the side group, and the DF comes from polymer backbone as a result of triplet-triplet annihilation. Efficient triplet energy transfer in the polymer films has been revealed by PL quenching method using doping the polymer films with different triplet acceptors and organometallic complexes. We argue that the exceptionally strong Ph in this polymer results mostly from a greatly increased ISC rate due to the latter occurs in this polymer between S_1 and T_1 states of different (viz., sigma and pi conjugated) parts of the macromolecule. This suggests a new concept of strong enhancement of the ISC for efficient conversion of primary excited singlets into triplets in conjugated polymers without involving a heavy atom effect, while the rate of radiative T_1-S_0 transition remains here virtually unaffected. Finally we demonstrate that this polymer could be promising for application as host material in white-light emitting OLEDs due to rather high intrinsic triplet level.

THE SPECTRAL-LUMINESCENT CHARACTERISTIC OF POTENTIAL-SENSITIVE PROBES IN SOLVENTS OF DIFFERENT POLARITY AND ISOLATED HEPATOCYTES

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The influence of microenvironment on the fluorescence parameters of new squaraine probes has been studied. It has been found that solvent polarity coefficient decrease shifted fluorescence emission maxima of anionic derivatives SqSC2, SqSC4, SqSEt, neutral dyes SqC1, SqC2, SqC18 as well as polymethine dyes H-510 and D-307 towards red-area wavelengths, which allowed us to assess a probe microenvironment in cellular structures. It has been detected that unlike polymethine dyes, the squaraine probes get localized mostly in membrane regions with higher polarity. Their localization can be explained by charges of chromophore structure and is connected with charge distribution on membrane of live cells and the transmembrane potential value. It has been found that among all the dyes H-510 and SqSC4 were the most sensitive probes to transmembrane potential changes induced by some agonists in hepatocytes. Our study shows that SqSC4 is the most stable to photodestruction, which is crucial for long-term monitoring.

EVOLUTION OF RAMAN SPECTRA OF RIBONUCLEOSIDES CONTAINING PYRIMIDINE BASES UNDER DEUTERATION

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Raman spectra of two ribonucleosides containing pyrimidine bases, i.e., cytidine [1,2] and uridine and anomalous nucleoside 6-azacytidine [3] and their deuterated analogs, were analyzed in solid state, in an aqueous solution and theoretically calculated. Analysis of all these spectra, measured on both native and deuterated species, allow us to present new interpretation of high frequency shift of some Raman peaks in the spectra of studied compounds. As deuteration affects not only eigenfrequency of vibrational mode but also set of displacements of nuclei involved in that mode so this may lead to increasing or decreasing of corresponding Raman peak's intensity. There is a possibility that there is no real high frequency shift of eigenfrequency of particular vibration mode but an apparent shift arising from drastic redistribution of Raman intensities of adjacent mode. To confirm this assumption the calculation of the vibrational spectra of studied compounds for different hypothetic hydrogen isotopes with atomic mass in range $1 \leq m_H \leq 2$, i.e. intermediate between hydrogen and deuterium, were made in order to monitor an evolution of the Raman spectra. It was turned out that there are no high-frequency shifts of Raman peaks under deuteration but change of relative intensity of the two adjacent modes takes place: namely an intensity of low-frequency mode decreases while intensity of high-frequency mode increases. Correlation calculations are also proving this assumption.

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THE SPECTRAL PROPERTIES OF ORGANIC POLYMERS AND FUNCTIONAL MACROMOLECULES DESIGN FOR PHOTONICS APPLICATIONS

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The main electronic processes in organic synthetic and biological polymers were examined. The investigations results of the peculiarities of the optical absorption, excitation energy transfer by singlet and triplet excitons, and resulting fluorescence and phosphorescence in these media were presented.

The number of possible applications of results obtained was examined. Particularly the answer on the question "How knowledge of the peculiarities of electronic processes in polymers can be used in design of functional polymers?" was done. It was discussed the applications in: molecular electronics; information recording; intramolecular plastification; the design of materials for OLEDs; aging and degradation of polymer materials (including problems of stabilization of polymers and protection of polymers against photochemical reactions).

The problems mentioned above were examined for biological objects too.

CLASSIFICATION OF BIOLOGICAL MACROMOLECULES: VISUALIZATION IN FORM OF GRAPHS AND TREES

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A novel discrete mathematical approach and corresponding software, called Boolean analysis or BOOL-AN is proposed as an additional tool for molecular systematics. The method is based on algorithms generating mathematical representations directly from DNA/RNA or protein sequences, followed by the output of numerical and visual (graphs, trees) characteristics. The binary encoded sequence information is transformed into compact analytical form, called the Iterative Canonical Form (or ICF) of Boolean functions, which is used as a generalized molecular descriptor. What is important, the basic requirements, formulated earlier for chemical codes are satisfied by the proposed molecular codes and molecular descriptors. They are unique, compact and complete, that is allow reconstruction of the sequence information without loss. Thanks to these features, the proposed generalized molecular codes and molecular descriptors can reveal the inherent abstract structure of the nucleotide or protein sequences, characteristic to the given biological function.

The method of classification, based on ICF-graph distance calculations is not restricted to relatively small molecules and can be used therefore for studying any DNA/RNA or protein sequences available in the current databases. As it is shown on samples of evolutionarily or functionally more related tRNAs the topology of macromolecules represented in form of ICF graphs is very similar, whereas it differs substantially for distantly related species.

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SPECTROSCOPIC STUDY OF IMIDAZOPHENAZINE-PENTADECATHYMIDILATE CONJUGATE AND ITS COMPLEX WITH POLY(DA)

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The end modification of the oligonucleotides by the intercalative dyes is widely used in antisense oligonucleotide technology to increase the stability of their complexes formed with complementary target oligo- and polynucleotides.

In our work imidazophenazine dye was attached to 5'-end of $(dT)_{15}$ oligonucleotide via flexible linker (Fig. 1).
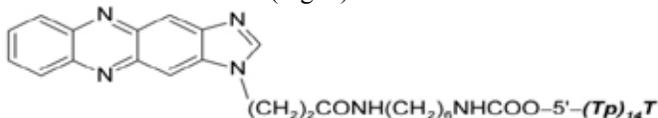
Fig. 1. Molecular structure of imidazophenazine-pentadecathymidilate conjugate.

Absorption and fluorescent properties of the constituents, as well as their changes in consequence of the conjugation were registered. Binding of $(dT)_{15}Pzn$ to synthetic poly(dA) was studied in 2.5 mM cacodylate buffer (pH 6.9) with 0.5 mM EDTA in the presence of 0.1 M NaCl using absorption, fluorescence and melting techniques. It was established that the duplex formation is accompanied by substantial absorption hypochromism, 2.5-fold fluorescence quenching, increase in fluorescence polarization degree and small opposite shifts of the dye spectral bands, which amount to 3 nm for absorption, and 4 nm for fluorescence one. The UV-melting profiles of poly(dA)·$(dT)_{15}Pzn$ were compared with those for non-modified poly(dA)·$(dT)_{15}$ obtained under the same experimental conditions. It was established that the modification of $(dT)_{15}$ by imidazopenazine results in the rise of the duplex helix-to-coil transition midpoint temperature of about 4.5 ºC. Such increase of the duplex thermostability is conditioned by an intercalation of planar imidazophenazine chromophore between nucleic bases. The changes of the thermodynamic characteristics, such as standard enthalpy, entropy and Gibbs free energy, were estimated in the frame of all-or-none model. It was shown that the tethering of the imidazophenazine to the 5'-end of $(dT)_{15}$ stabilizes the duplex formation increasing the value of standard Gibbs free energy change by 1.3 kcal/mole per oligonucleotide strand or 0.087 kcal/mole per AT-pair.

SPECTROSCOPIC STUDY OF THE INTERACTION OF CATIONIC PHENAZINE DERIVATIVES WITH INORGANIC POLYPHOSPHATE

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The weak electrostatic interaction of the cationic dyes with the external surface of DNA double helix is known to be exists along with the strong intercalative mechanism. The contribution of this interaction type into the complex formation is essential due to the cooperative character of the binding. It should be considered to determine correctly the intercalation characteristics such as binding site number, their specificity or the process cooperativity. It is known that several phenazinium salts forms both intercalative and external complexes with DNA. In the present work the binding of three phenazine derivatives, namely N5-ethyl-β-pyrrolidono(4, 5-d)-phenazinium perchlorate (F1), 3-(1-prolyl)-N5-ethyl-phenazi-nium perchlorate (F2), and 3-(alanyl)-N5-ethyl-phenazinium hydrosulfate (F3), with inorganic sodium polyphosphate (PPS) was studied by several spectroscopic methods. Absorption and fluorescent properties of the complexes were precisely determined in a wide range of molar polymer-to-dye ratios (P\D). Measurements were carried out in aqueous buffered solutions under low ionic conditions. No changes in absorption and emission characteristics of dyes were observed under P\D variation. Both fluorescence intensity and fluorescence polarisation degree were practically without changes. To explain this fact, it is possible to suggest that the zvitterionic structure of F1 and F2 derivatives hinders their complex formation with PPS chain. Whereas the binding of monocationic F3 derivative to polyanionic chain of inorganic PPS was expected to be observed. The absence of features in the absorption spectra pointing out to the chromophore stacking-association can be explained by deficient shielding of the chromophore positive charges.

PECULIARITIES OF PYROACTIVITY IN PVDF BASED POLYMER, COPOLYMER AND COMPOSITE FILMS

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Polar films of polyvinilydene fluoride PVDF and its copolymers P(VDF/TrFE) with trifluoroethilene (TrFE) are intensively used for piezo- and pyroelectric sensors and bending actuators, which operation parameters in high degree are determined by remanent polarization P_r, and so by space distribution of polar characteristics, in particular by profiles of pyroactivity distribution (PPD).

The PPD was examined for PVDF and P(VDF/TrFE) films of various production ("Solvay"- Belgium, "Piezotech"- France, "Kureha" - Japan, "Plastpolymer"- Russia, "Pennwalt"- USA) and ferroelectric crystal – polar polymer TGS-P(VDF/TrFE) composite films. The study of PPD was performed by photothermomodulation pyroelectric method in the pyroelectric current mode ($U_\pi = U_{\pi 1}$ µ γ/c_1, $\gamma = dP_r/dT$ is the pyroelectric coefficient, c_1 is the volume heat capacity) and pyroelectric voltage mode ($U_\pi = U_{\pi 2}$ µ $\gamma/c_1 \varepsilon$, ε is the dielectric permittivity) in modulation frequency f_m range 1 Hz $\leq f_m \leq$ 100 kHz.

For the edge fixed films the pyroelectric resonance (PyR) and antiresonance (PyAR) regions were observed in f_m-range 1-10 kHz corresponding to λ_T-range of 1.5-4 µm ($\lambda_T = (a_T/\pi f_m)^{1/2}$, a_T is the thermal diffusivity). Such PyRAR phenomenon was proved to be connected with bending vibrations through the thermal expansion coefficient α_1 and piezoelectric module d_{31}.

The inversion of the sequence of the resonance f_r and antiresonance f_a frequencies from usual ($f_r < f_a$) (PyRAR) to inversed ($f_a < f_r$) (PyARR) under excitation of the film sides being at different signs during poling was found and connected with specifics of space charge state under the electrodes.

The direct relation of PPD shape and the PyRAR phenomena was

manifested for spin coated corona charged films of TGS-P(VDF/TrFE) with 5 μm-powder of LA doped TGS single crystal. Indeed, PyRAR(ARR) regions observed in the films with non-uniform PPD disappeared after additional d.c. poling resulted in more uniform PPD.

PyRAR phenomenon is considered as consequence and indicator of pyroelectric, piezoelectric and space charge under-surface inhomogene-ities. PPD controlling and application prospects are discussed.

THE SPECTRAL PROPERTIES OF NEW DYES FOR PHOTONICS APPLICATIONS

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The design and creation of low-energy expenditure sources of light is one of the main problems (caused by the energy crisis) of the modern technology world at the last time and requires new scientific solutions. The promissory variant of this problem solution is the usage of organic dyes with the luminescence high quantum yield for the creation of Organic Light-Emitting Devices (OLEDs). The materials used for such devices construction have to be stable and easy excitable by light or electrical current without excitation the materials used as matrix for these dyes. In the present work the characterization by spectrum-optical methods of the series of new dyes were done.

The optical absorption and fluorescence spectra of the films (embed in poly-tetrafluoroethylene (PTFE) matrix) and solutions (in a number of organic solvents) of the series of new malonocyanine dyes (dihydropyrimidine derivatives titled 2565, 2566 and 2900) with isolated unsaturated groups have been investigated. For 2565 and 2566 dyes solutions the optical absorption spectrum band that corresponds to the first electronic transition is observed in the spectral range near 420 nm and the fluorescence spectrum band is observed near 440 nm. For 2900 dye solution there are four absorption spectrum bands (390, 470, 570, 670 nm) that correspond to the first transition; the fluorescence spectrum band (under excitation by light with wavelength 405 nm) is observed near 450 nm. The correspondent spectra bands for 2566 dye films are shifted on ~20 nm relative to the solutions spectra bands. For 2565 and 2900 dyes only the optical absorption spectrum band near 450 nm is observed and no fluorescence spectrum band (under excitation by 405 nm) is observed. In the range 250-350 nm that corresponds to the optical absorption of the majority of the synthetic and biological polymers (including PTFE) no absorption spectra bands of 2565, 2566 and 2900 dyes were observed. This fact gives the possibility to excite these dyes molecules without the exciting of a matrix polymer. So, taking into account the facts mentioned above 2566 dye is proposed for the organic light-emitting devices creation.

EFFECTS OF PHOTOCONDUCTIVITY AND PHOTOLUMINESCENCE IN THE FILMS OF POLY-N-EPOXYPROPYLCARBAZOLE WITH ANIONIC POLYMETHINE DYE

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The films of polymeric composites (FPC) doped with the organic dyes are widely used in information recording and electroluminescent mediums, as well as in photoelectric converters of solar energy. The dye molecules, for example polymethine, are employed as the centers of light absorption and photogeneration of non-equilibrium charge carriers. In the solid polymeric matrixes polymethines show tendency to association. Influence of external electric field on the spectra of absorption, photoluminescence, electric and photoconductivity of the films of poly-N-epoxypropylcarbazole (PEPC) doped with anionic polymethine dye based on malononitrile is investigated in the present work. Molecules of the dye in the excited state are able to yield electron but are not able to capture it. However, increase of quenching of photoluminescence intensity in the external electric field, appearance of long wave band of photoluminescence and effect of photoconductivity are observed in FPC when the concentration of the dye increases. It was demonstrated that associates of "sandwich" type of the dye structure arise in FPC when the concentration of anionic dye is increased. Intercombination conversion intensifies in these associates. Convergence of energy of high occupied orbitals of the associates and carbazolile fragments of PEPC happens due to splitting of energetic level of excited state of the associate. This convergence opens possibility for transport of non-equilibrium holes through carbazolile fragments of PEPC as well as for transport of electrons inside and between the dye associate in singlet and triplet states.

THE HIGH-EFFECTIVE SENSOR WITH OPTICAL RESPONSE ON THE PHENOL MOLECULES PRESENCE IN WATER POLLUTED BY OIL

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The purification of natural water polluted by oil and its hazardous components is one of the main tasks of the modern scientific world. It is known that even low concentrations of molecules of some oil components are very toxic. One of such components is phenol that is high-soluble in water. That is why the development of new high-effective principles, methods and equipments of such molecules (like phenol) detection and extraction from water is the very actual task. In the present work the applying of optical methods to phenol express detection were examined.

The phenol molecules manifest strong absorption at 280 nm and fluorescence at 300 nm. This gives the ground to apply the optical methods for phenol direct detection. To the other hand, for the detection of extremely low concentration of phenol molecules the using of methods of some phenol molecules previous accumulation is required. One of the variants of this task solution is the usage of functional polymer macromolecular complexes with optical response and chemical structure that allows the non-native impurities to be sorbed from environment and easily detected by the optical spectroscopy methods. For this purpose the intramolecular polymer complex based on poly(vinylalcohol) with poly(acrylamide) grafted copolymers (PVA-PAA$_N$) that posses such properties was used. In the present work the results of PVA-PAA$_N$ sorbtion properties investigations by the optical spectroscopy methods were described, the mechanisms of sorbtion were discussed, and efficiency of purification of natural water by PVA-PAA$_N$-films was examined. It was shown the molecules of some organic compounds are sorbed by PVA-PAA$_N$ effectively. The highest adsorbtion rate was found for phenol molecules. The data obtained give the possibility to create the high sensitive sensors with the optical response for detection (and concentration measurements) of the phenol molecules from water polluted by oil products. Besides, the mentioned above copolymer can be used for effective purification of natural water polluted by oil.

COMPARISON OF HYDRATION OF OXYETHYLATED DERIVATIVES OF ACETAMIDE AND GLYCEROL

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Nowadays, oxyethylated derivatives of acetamide (OEA) in parallel with oxyethylated derivatives of glycerol (OEG) are actively investigated as very promising cryoprotectants. It is obvious that the effectiveness of a cryoprotectant correlates significantly with its ability to form hydrogen bonds with water. It prevents or reduces formation of the hexagonal crystal lattice of ice which causes damage of biological objects during a process of cryoreservation. We have determined the hydration number of OEA molecules having the polymerization degree of $n = 1$ and 7-8 on the basis of analysis of phase diagrams constructed using the DSC data. It has been shown that about 8 water molecules bind to an $OEA_{n=1}$ molecule, and about 32-33 water molecules bind to an $OEA_{n=7-8}$ molecule. Previously, we determined the hydration number of molecules of OEG having the polymerization degree of $n = 5$, 25 and 30 using the methods of DSC and IR-spectroscopy [1, 2]. It was shown that each element of the polymeric chain can bind to about 3 water molecules. Having compared the hydration numbers of these two homologous series of the polymers, we can say that the effectiveness of oxyethylated acetamide as a cryoprotectant is determined by high glass-forming tendency due to the presence of hydrophilic groups in both oxyethyl units and an acetamide molecule.

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EFFECTS OF UV RADIATION UPON PHASE TRANSITIONS IN HYDRATED PHOSPHOLIPID SYSTEMS CONTAINING PHOTOSENSITIVE MOLECULES OF BIOLOGICAL ORIGIN

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Recently [1, 2] a new bioequivalent sensor material for UV detection and dosimetry was developed. It based on cholesteric liquid crystal (CLC) doped with a photo-active molecules of biological origin – provitamin D, capable to UV-induced photoisomerisation leading to formation of vitamin D. This process leads to the changes of macroscopic parameters of CLC matrix such as maximum selective reflection wavelength (λ_{max}) and mesomorphic phase transition temperatures.

It is well known that in living organisms biosynthesis of vitamin D from the provitamin D takes place in membranes of epidermal cells, so the aim of the present work was to study provitamin D photoisomerisation process in a model membrane system based on lamellar phases of hydrated phospholipids.

Using differential scanning calorimetry (DSC), it was shown that UV-induced photoisomerisation of provitamin D resulted in changes of phase transition temperatures in hydrated phospholipid systems. The character of the changes was essentially similar to that observed in cholesteric systems, reflecting the changes in molecular structure of the photosensitive substance acting as a non-mesogenic dopant. This is considered as a direct biophysical argument confirming the bioequivalence of the developed sensor material for UV dosimetry.

In another set of experiments, similar studies were carried out for hydrated phospholipid systems containing one more human UV chromophore – urocanic acid. In this case, effects of UV radiation on phase transition temperatures were also noted.

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SPECTROSCOPIC STUDIES OF MOSQUITO IRIDESCENT VIRUS, ITS MAIN CAPSID PROTEIN AND DNA

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Mosquito iridovirus (MIV) is a DNA-containing icosaedric cytoplasmic virus which affects mosquitos of *Aedes, Culex, Culizeta* genera. Apart from mosquitos and other insects, iridoviruses cause mass death of fish and cause huge losses for industrial fish breedings. The MIV particle consists of a core of genetic material (double-stranded viral DNA), surrounded by a capsid (icosahedral protein shell) and further encased in a lipid envelope.

The aim of the work was to identify aromatic amino acids (tryptophan, tyrosine and phenylalanine) which are supposed to be present in the MIV's major capsid protein by means of optical spectroscopy and to model the capsid protein spectra with a combination of spectra of separate amino acids as well as to model the MIV spectra with a combination of spectra of separate amino acids and viral DNA.

Measured are absorption, fluorescence, fluorescence excitation and phosphorescence spectra of MIV, its major capsid protein and viral DNA dissolved in TRIS-HCl, TRIS-HCl-EDTA buffers and distilled water, respectively, as well as absorption and fluorescence spectra of the three amino acids dissolved in distilled water (tryptophan, tyrosine and phenylalanine).

From absorption, fluorescence and phosphorescence spectra it is found that MIV capsid protein contains all three mentioned above anino acids (tryptophan, tyrosine and phenylalanine) in different proportions. MIV phosphorescence spectrum at liquid helium temperature is found to be well described as a linear combination of phosphorescence spectra of its components (the three amino acids and viral DNA). Contribution of phosphorescence spectrum of each amino acid was determined by its relative content in virus capsid protein and phosphorescence quantum yield.

BERBERINE AND SANGUINARINE INTERACTION WITH DNA: SPECTRAL MANIFESTATIONS AND BINDING PARAMETERS

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Isoquinoline alkaloids belong to a group of plant metabolites; they are widely used in medicine as both itself and the components of pharmacological drugs. Among them, berberine and sanguinarine are very important. Both alkaloids possess antimicrobial, anti-inflammatory, antitumor properties. These medicinal activities are attributed to their ability to form a molecular complex with DNA. In this report, we present some spectroscopic aspects of sanguinarine and berberine binding with the DNA.

The absorption, excitation and fluorescence (PL) spectra of alkaloid and alkaloid+DNA solutions have been obtained for the P/D (the DNA base pairs/drug) values of 0…20. The binding of alkaloid to DNA was characterized by changes of the extinction coefficient (hypochromism) and the red shift of absorption maxima in the absorption spectra, blue shift and changes of the intensity in PL spectra. The remarkable increase (up to 200 times) of the berberine PL intensity takes place. On the contrary, the sanguinarine fluorescence intensity decreased by the complex way when the DNA is added. All these facts indicate the formation of the DNA-alkaloid complex. It was shown that the binding way depend on P/D. The parameters of berberine and sanguinarine binding with DNA were determined using the modified Scatchard and McGhee-von Hippel equations. For convenience these equations were transformed for direct use of experimental data. Such conversion gave opportunity to avoid Scatchard plot building procedure which is too sensitive to experimental data precision and involves uncontrolled error even for fair data.

Berberine. To interpret experimental data the McGhee-von Hippel equation for cooperative binding was applied. On the base of used approach binding parameters were obtained: $K = (5.2\pm0.2)\ 10^4\ M^{-1}$ (binding constant); $n = 2$ (number of binding sites covered by alkaloid mol-

ecule); $w = 1.3\pm0.2$ (co-operativity parameter). On the base of obtained results it can conclude that the most probable way of binding is an inter-calation of alkaloid molecules between DNA base pairs.

Sanguinarine. The model of two binding modes (external binding, small values of P/D≤1 and intercalation, P/D≥2) was applied for ex-plaining of the experimental results. A system of the binding way-de-pended equations of Scatchard and McGhee-von Hippel was used. The obtained parameters for an iminium form: $K_1 = (3.5\pm0.3)\ 10^5\ M^{-1}$ (exter-nal binding); $K_2 = (1.1\pm0.4)\ 10^6\ M^{-1}$ (intercalation), $n = 1.5$.

THE FUNCTIONAL MACROMOLECULAR COMPOUNDS BASED ON CARBAZOLE, PHENOTHIAZINE AND INDOLE FOR PHOTONICS APPLICATION

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One of the main problems of the modern technology world is the development of alternative energy sources and effective low power light sources. The solution of this problem stimulates investigations of the materials that could be used as an active medium in photo-electric cells (solar cells) and electroluminescent devices (so-called LEDs, OLEDs and OPhEDs). In this paper the results of the spectral investigations of the functional macromolecular compounds containing carbazole, phenothiazine and indole pi-electron systems (specially designed for electroluminescent devices production) are presented.

The spectral properties (optical absorption, fluorescence and phosphorescence) of these compounds in solutions and powders at 293K and 77K were studied. The positions of the first singlet and triplet electronic energy levels of the compounds were evaluated; the schemes of electronic processes in corresponded bulk materials caused by initial chromophore excitations were proposed. The obtained data prove that substantial efficiency of intercombinatory conversion into the triplet state at 77ºK is typical for the most of the investigated compounds. The delayed emission of two investigated carbazole-containing compounds corresponded to the fluorescence band is, in our opinion, the delayed fluorescence that points to the triplet excitations migration in these compounds at 77ºK. The presence of the delayed fluorescence observed for these carbazole-containing compounds in bulk form proved the effective triplet excitations migration with their following annihilation. The position of the fluorescence and phosphorescence bands allows us to consider investigated compounds as potential chromophores for OLED/OPhEd applications.

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THE SPECTRAL TESTING OF THE INTERACTION BETWEEN PROTEINS AND POLYNUCLEOTIDES

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The oligonucleotides and ribonucleic acids are the biological compounds contained in the cells of all living organisms. Because of the natural origin of these compounds the drugs based on them become widely used last time in clinic and research medicine. Artificial synthesized oligonucleotides that bind to a specific target molecule (for example, protein) – aptamers – are being tested clinically just now as the cures for the diseases of blood, eyes, as immunomodulators, antivirus and anticancer drugs. The electronic properties of these compounds as well as some proteins are manifested in the optical (near biologically active ultraviolet, visual and near infrared) range. This gives the ground to apply the optics spectroscopy methods for the investigations of electronic structure and interaction between oligonucleotides / ribonucleic acids and proteins.

In the present work the possibility of application of a low-temperature autoluminescence method for the detection of the binding between biological objects was studied. The positions of the first excited singlet and triplet electronic energy levels of the ribonucleotides were specified and the same positions of π-electron containing amino acids were evaluated using absorption and luminescence spectra. The spectral evidences of the binding between human albumin molecules and oligonucleotides / ribonucleic acid molecules were obtained. One of the important evidence of the albumin-2'-5'A$_3$ binding is appearance of the sharp structure in the phosphorescence structure under the T=77K (under these conditions phosphorescence spectra of separate 2'-5'A$_3$ is almost structureless).

NATURE OF FLUORESCENCE AND COLOURING OF POLYTETRAFLUOROETHYLENE TREATED BY Γ-IRRADIATION NEAR THE MELTING POINT

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Polytetrafluoroethylene (PTFE) is a widely used material due to its unique properties, such as excellent chemical and thermal resistance, biological stability, dielectric properties, antiadhesive properties, its low coefficient of friction, and its low thermal conductivity in combination with good viscous-elastic characteristics at low temperatures. Among the disadvantages of PTFE are high creep coefficient, low wear resistance (mainly at low temperatures) and extraordinarily low radiation resistance, which play relevant role when such material applied in the nuclear power plants or in spacecrafts. To improve these characteristics the modification of PTFE by radiation treatment in melting state has been used. Earlier we have shown that PTFE subjected to γ-irradiation under this condition gains color and fluorescent properties [1,2].

In the present work the spectrophotometric and spectral luminescence investigations of the γ-irradiated near its melting temperature PTFE film and block samples have been performed. Absorption and fluorescence characteristics of the optical centers formed in irradiated PTFE have been obtained. It was determined, that the different optical centers are responsible for the fluorescence behavior and coloration of the irradiated PTFE. The fluorescence optical centers are the conjugated polyen structures in a polymer chain. The coloring centers are the low-molecular fluorine-containing compounds liberating from heated up PTFE during process of a γ-irradiation. They interact with an uncontrollable impurity, which present in argon gas, and also with a products allocated on the chamber walls. Some of the formed compounds are colored. They are adsorbed on a surface of PTFE samples and give them certain color. The fluorescent structures are formed both at a near-surface layer and in bulk of a sample. Their concentration slightly changes at the various dosage of gamma-radiation (which ranged

from 0.2 to 0.8 MGy), while the concentration decreases notably with a deepening into sample. It was confirmed, that the molecular oxygen traces in a sample play an important role in formation of the optical emission centers.

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PIEZOELECTRIC CHARACTERISTICS OF PYROELECTRIC DETECTOR OF LASER RADIATION ON THE BASE OF PVDF POLYMER FILM

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High values of piezoelectric coefficients (the order 30pC/N) of polyvinylidene fluoride (PVDF) ferroelectric polymer films testify to possibility of origin of electric fields in conditions when these materials are exposed to influence of vibrational and acoustic fields. These influences import precisions to process of measurement of a signal of the pyroelectric response (the primary contribution) U of radiation detector, which created on the basis of the PVDF ferroelectric film, at absorption both coherent, and incoherent radiation from researched object. These precisions cause presence of a spurious signal (the secondary contribution) in the pyroelectric response of radiation detector (RD).

A distinguishing characteristic of the PVDF films is temperature dependence of piezoelectric coefficients, and also influence of this dependence on the secondary contribution. Now temperature dependence of these piezoelectric coefficients is insufficiently studied, and the data about its influence on the secondary contribution in pyroelectric response in the science literature practically misses.

The purpose of this work was research of temperature dependences of values of piezoelectric coefficients d_{31}, d_{32} and d_{33} of polymeric PVDF films for the purpose of optimization of operation the RD on the basis of this material.

The polymeric films of the thickness $l = 110\mu m$ were used in experiments. These films have been produced by company *Precision Acoustics LTD (PAL)* (Great Britain). These films had the high content of ferroelectric β-phases and they had gold electrodes, which were coated in vacuum. Films have been placed in a temperature cell which allowed to change temperature in limits from room to 90^0C.

Measurements of piezoelectric coefficients d_{31}, d_{32} and d_{33} were led by a static method in a temperature cell in a mode of direct piezoelectric effect at which the electrical charge arose on electrodes both at expanding, and at

compressing pressure. In these experiments the value of strain σ didn't exceed value 300MPa.

The obtained temperature dependences of these piezoelectric coefficients represented non-monotone dependences $d_{ij}(T)$.

Values of temperature dependences of pyroelectric response signals U(T) in the conditions of acoustic influences have been measured and at different methods of fastening of the PVDF films on holders.

On the basis of obtained experimental and theoretical data the inference has been drawn on conditions of optimization of the RD operation for the purpose of reduction of influence of the secondary contribution in pyroelectric response.

NEGATIVE PHOTOCONDUCTIVITY OF FERROCENYL CONTAINING OLIGOMER FILMS WITH A MEROCYANINE DYE

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Films of polymer composites (FPC) containing ferrocene derivatives $(Fe(C_5H_5)_2)$ can ossess photosemiconducting properties. Such polymer composite films are attractive for application in information media. Photoconductivity of FPC in the visible light region is provided by additives of organic dyes, whose molecules after absorption of light energy are capable of photogeneration of nonequilibrium charge carriers. The effect of negative photoconductivity of ferrocenyl_containing oligomer films doped with a merocyanine dye based on ferrocene and tetranitrofluorene has been found. The decrease in the conductivity current and its recovery after switching off light are in agreement with the decrease and the recovery of the dielectric loss tangent in the films studied. The discovered effect of negative photoconductivity of FPC based on ferrocenyl_containing oligomer can be due to significant unevenness of the spatial distribution of the fragments over which the transport of nonequilibrium charge carriers occurs. We may suppose that such spatial unevenness of the distribution of the fragments is determined by structural features of oligomer molecules, namely, proximity of the lateral fragments within the molecule and long distance between them in the adjacent molecules. In this case, transport of nonequilibrium charge carriers among adjacent molecules is hindered as compared with their transport within the separate molecule, and this creates the conditions for the formation of electrically charged centers with a long lifetime and low mobility of charges on them. Such electrically charged centers are the reason for the decrease in the electric field operating in FPC. The phenomenological model is suggested in which the buildup of space charge from nonequilibrium current carriers and its effect on electric conductivity of the films are taken into account.

POLYMER COMPLEXES WITH LITHIUM BONDING:SPECTRAL ASPECTS

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Polymer complexes occur with different kinds of bonding, mainly with hydrogen and ionic bonds. Lithium bonding is more rare in general [1], it is possible between Li-ion and oxygen or nitrogen atoms in organic compounds and it is completely analogous to hydrogen bond:

X-Li...Y (Y =O or N) It was also supported by CNDO calculations [1].

Regular polymers, e.g. polyethylene oxide, can form ordinary Li complexes with coordination bonds and it reflects in their NMR- and IR-spectra [2]. These complexes are formed between Li-ion of lithium salts and oxygen atom in the main chain of polyethylene oxide . Due to them films of such polymers have ionic conductivity and can be used as solid electrolytes for lithium batteries [2].

Firstly it had been shown by us that oxygen atoms in the side chains can also participate in complex formation, e.g. as in copolymers butyl vinyl ether – acrylonitrile (new bands in IR spectra). Recently new irregular copolymers of acrylonitrile were synthetized and characterized using as comonomers butyl-, hexyl-, octyl- and nonyl- methacrylates in different comonomers ratio. These copolymers were used as models for studying the influence of functional groups and component polarity on dielectric parameters and conductivity values, as well as complex-formation abilities, and estimated by the dielectric and the NMR-spectroscopy methods. Dielectric measurements were carried out over the temperature range of 120-411 K and the frequency range of 0,7-15 kHz. The dielectric characteristics (dielectric constant ε', dielectric loss tgδ, loss factor ε'' and effective conductivity σ) were measured using copolymer films with a thickness of 1,5-2,0 mm and a diameter of 25 mm.

The NMR spectral data as well as dielectric studies demonstrate complex-formation between Li-ions and O- or N-atoms in copolymers. These interactions can be observed due to lithium bonding in such systems.

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ZN²⁺ ION EFFECT ON DNA TRANSITION INTO METALLIZED FORM IN ALKALINE SOLUTION

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Interest in studies of structural and thermodynamic properties of DNA metallized form is caused with a possibility of its using as nanoelectronic and nanobiosensory elements [1-3].

The method of differential UV-spectroscopy was applied to study peculiarities of effects of Zn^{2+} ion concentration on B-DNA transition into the metallized form in the whole range of temperatures of the double helix existence (from 25 ^{0}C to 70 ^{0}C) in solutions containing 0.01 M Tris-buffer (pH 8.5), 0.005 M NaCl and variable concentrations of $ZnCl_2$. It was revealed that Zn^{2+} ions induce hypochromicity of the whole absorption spectrum of DNA the limit value of which in the DNA absorption maximum runs up to 24 %, and this corresponds to the metallization degree [m] = 100 %. The last is realized only upon heating of solutions being of $[Zn^{2+}] \geq 2 \cdot 10^{-4}$ M concentration. For the first time, the phase diagram has been obtained for DNA-zinc complex, being composed of regions with different characters of [m] dependence on temperature and Zn^{2+} ion concentration.

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CHEMICAL IMAGING OF RENAL STONES BY MEANS OF INFRARED SPECTROSCOPICAL MAPPING

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Renal stone disease is a very common disease, occurring in both industrialized and developing countries and mainly affecting adults in a very broad age range (20–60 years). The formation of kidney stones is a process influenced by many factors. Primary contributing pathogenic factors are genetic, nutritional and environmental, also personal habits could be of some importance. Information about the chemical structure of kidney stones is crucial to the treatment and prevention of the kidney diseases. Unfortunately, universal method sufficient for providing all the clinically useful information about the structure and composition of the stones is not available up to date. Infrared spectroscopy is showing a grate potential in the field of renal stones analysis. Recent advances in infrared imaging technique allow not only investigate chemical composition of the sample, but also obtain detail information on spatial distribution of the chemical components in the sample.

The stones for this study were surgically removed from patients in Urology centre of Vilnius University hospital 'Santariskiu Clinic'. The stones used for the mapping were cross-sectioned and polished in order to get as good as possible specular reflection from the sample. The imaging is performed using reflected infrared light. Specular reflection exhibits absorptions resembling the first-derivative of a conventional absorption spectrum. Intensity of these *Reststrahlen* bands is proportional to concentration of particular chemical constituent of the stones. False-color images representing the distribution of different chemical components in the urinary stones were obtained by integrating the area under the spectral band of specific chemical component.

LUMINESCENCE OF URACIL MOLECULES UNDER THE INFLUENCE OF ELECTRON IMPACT

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The article deals with the results of experimental investigations of excitation process in uracil (as the base of nucleic acid) by low-energy electrons. These investigations continue our previous ones, which were made for the other bases of nucleic acids – cytosine and thymine [1,2].

The experiments were tried through optical method that we had used earlier [2]. In the investigations, there was used the uracil preparation in the form of polycrystalline powder of Sigma-Aldrich Firm. Formation of gas phase of uracil took place through its heating in a separate metal container. The formed gas phase of uracil entered the cell through the steam conductor. The temperature of the container with uracil powder did not exceed 350 K The electronic beam was formed by the five-electrode gun with a tungsten cathode. The cell was located in the magnetic field in such a way that its force lines were parallel to the electronic beam. The magnetic field induction was equal to $\sim 1.2 \cdot 10^{-2}$T. The experiments were tried at the following conditions: the current strength of the electronic beam was in the range of $(3-4) \cdot 10^{-5}$ A, the electron energy spread (FWHM) being $\Delta E_{1/2} \sim 0.5$ eV, the vacuum degree was $\sim 1 \cdot 10^{-5}$ Pa.

In the investigations that were made, there were obtained emission (luminescence) spectra of uracil in the wavelength range of 200 – 500 nm for different energies of the exciting electrons. In these spectra, there are manifested two wide molecular bands that we identify with the radiation of singlet and triplet state of uracil molecule. Such an interpretation does not contradict to our calculations that were made through the semi-empirical method AM1 of the program package HyperChem 8.0. In the spectra, there are also manifested at 100 eV electron energy ten molecular stripes whose maximums are at the following wavelengths: $\lambda_{M}\lambda_{M}$ = 286.5; 307.5; 317.2; 333.2; 369.6; 408.1; 432.0; 482.2; 525.0 nm. In our opinion, these additional bands reflect the dissociative excitation of uracil molecules.

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NIR BODIPY DYES WITH CYANINE-LIKE SUBSTITUENTS AND NATURE OF THEIR ELECTRON TRANSITIONS

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The dyes derived from boron dipyrromethene (4,4-difluoro-4-bora-3a,4a-diaza-s-indacene, BODIPY) have attracted considerable attention because of their excellent thermal, chemical, and photochemical stability, high molar absorption coefficients, high fluorescence quantum yields, general insensitivity to both solvent polarity and pH, large two-photon cross-section for multi-photon excitation, the lack of ionic charge, and a good solubility. However, most BODIPY compounds have absorption maxima below 600 nm. As long-wavelength dyes are important for both basic and applied research, there are many synthetic approaches for modifying the BODIPY system so as to red-shift its absorption. One of the most promising approaches to the modification of BODIPY is its peripheral functionalization at meso- and α-positions with conjugated chromophores.

More effective might be the introduction of complex heterocyclic residues, which are the end groups in cyanine dye. They are characterized by highly intense and highly selective absorption, which covers the spectral region from ultraviolet to near infrared wavelengths by a polymethine chain length changes and changes in "effective length" of finite residues.
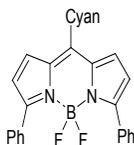
1a X = C(CH₃)₂ **1b** X = S

1c X = CH=CH
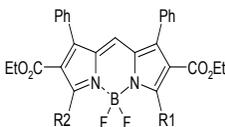
2 R1 = CH₃, R2 = Cyan

3 R1 = R2 = Cyan
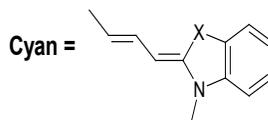
a X = C(CH₃)₂ **b** X = S

c X = CH=CH

A series of BODIPY-based dyes bearing one or two polymethine chromophores at their α-positions were prepared through condensation reactions of 3,5-dimethyl borondipyrromethene with various hemicyanines. The dyes obtained exhibit record deep absorption among known borondipyrromethene

derivatives (λmax up to 970 nm)
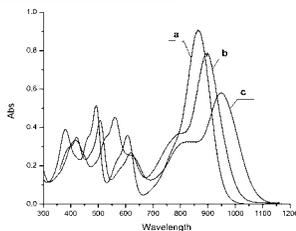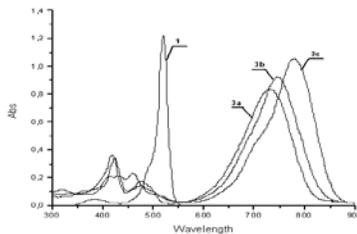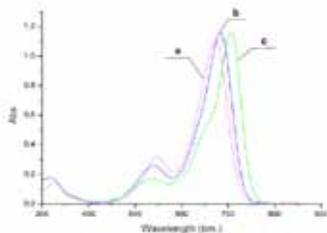
Absorption spectra of dyes 1a – 1c   Absorption spectra of dyes 2a -2c
Absorption spectra of dyes 3a – 3c

   To understand the nature of electron transitions in the BODIPY and its derivatives, the quantum-chemical calculations of the electron structure were performed. It was shown that introducing of two cyanine-like substitutients in *meso-,a`-*positions leads to the additional deeping of color by donor levels splitting.

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METHODS AND APPLICATIONS

POLARIZATION MEASUREMENTS IN FEMTOSECOND TIME DOMAIN

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Polarization measurements are among the most precise and sensitive in optics. A number of fine physical effects as well as analytic techniques are based on the variations of polarization of light. Polarization measurements are equally useful in time-resolved spectroscopy [1] and time resolved imaging. It should be noted that unlike spectral measurements the precision of polarization measurements does not decrease with increase of temporal resolution. However, certain technical issues and specific materials properties should be taken into account. For example, the best quality polarizers used in conventional optics – calcite polarization prisms – are not always good in the case of femtosecond pulses. Because of considerable difference of n_o and n_e polarization prism can cause substantial pulse broadening for large diameter beam. Large thickness of the prism also contributes to pulse broadening. Another case of polarizers – polymer polaroid films do not cause pulse broadening but they have poor stability in high intensity beams, they are easily bleached and even damaged. And quality of polarization provided by polaroid films often is insufficient for precise measurements. A novel type of polarizers – nanoparticle linear film polarizers provide much better quality (extinction ratio up to 10^5) and have rather high damage threshold.

An example of time-resolved polarization measurements performed in pump-probe experimental setup is presented. Optically induced anisotropy of surface plasmon in spherical copper nanoparticles is observed under irradiation by intense femtosecond laser pulse with power density 10^{11}-10^{12} W/cm^2. Subpicosecond kinetics of plasmon shifts and induced anisotropy may be useful for applications in optical switches and ultrafast sensors.

Another interesting application of polarization technique in femtosecon time domain is optical Kerr shutter for time-resolved luminescence measurements. Details of experimental setup, its characteristics, and requirements to optical elements will be presented in the report.

[1]. I. Dmitruk, I. Blonskiy, I. Pavlov, et al, Phys. Rev. B82, 033401 (2010)

ANALYTICAL METHODS STUDY OF WAVE FUNCTIONS AND ENERGY LEVELS OF EXCITED VIBRATIONAL STATES OF MOLECULES

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A method for investigating the excited vibrational states of molecules based on the analytical perturbation theory for linear operators is proposed. According to this theory, the similarity transformation of the total projector and the construction of the transforming function allow obtaining analytical representations of eigenvectors, and in the course of reduction, eigenvalues of the perturbed operator. Theoretical statements and formulas of contributions of analytical perturbations are applied to the investigation of vibrational–rotational interactions, determination of wave functions, and corresponding energy values of excited vibrational states of molecules. The perturbation theory or linear operators is closely related to modern theoretical physics. In the present paper, this theory underlies the solution of the fundamental problem of quantum mechanical theory of vibrations of molecules concerning vibrational–rotational interactions and provides obtaining analytical representations of perturbed wave functions and corresponding vibrational energy values.

The objective of this paper is to apply basic theoretical statements and results of analytical perturbation theory for linear operators to the construction of the holomorphic operator function $W_v(\varepsilon)$ and inverse function $Z_v(\varepsilon)$. These functions are used to perform similarity transformations of wave functions of the unperturbed vibrational Hamiltonian $\{\Psi_k, k = 1, 3N{-}6\}$ to sought wave functions of the vibrational–rotational Hamiltonian $\{\Psi_k(\varepsilon), k = 1, 3N{-}6\}$ for obtaining determining expressions for contributions of perturbations to wave functions and corresponding energy values of excited vibrational states of molecules.

In this paper, strict proof of the existence of analytical representations for perturbed wave functions and eigenvalues of vibrational–rotational Hamiltonian was obtained. Methods for determining the contributions of perturbations using the similarity transformation of projectors for eigenwavefunctions and the process of reduction for corresponding eigenvalues were proposed. Formulas to the *n*-th order of the perturbation theory giving the explicit expressions for elements of analytical perturbations of wave functions and energy values of excited vibrational states of multiatomic molecules were presented.

COMPARATIVE STUDY OF CRYSTAL AND POLYMER PHOTOACTIVE MEDIUMS FOR POLARIZATION HOLOGRAPHY

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Polarization holography has many unique properties and possibilities as compared to scalar holography. These ones result in advantages of polarization holographic information storage and in more flexible opportunities of light beam control when using light polarization sensitive photoactive mediums.

Polarization holography technique is based on registration of the polarization state of the total field of the reference and object light beams by the polarization sensitive recording mediums. Starting from discovery of holographic recording a lot of attempts of fabrication of polarization sensitive mediums were done. The aim of the present work is the comparative analysis of the features and potential possibilities of three polarization sensitive recording mediums: i) magnetic yttrium iron garnet doped with cobalt (YIG:Co); ii) CaMnGe garnet; iii) films of polymeric compositions (PC) containing azobenzene polycomplexes with coordinated cobalt ions. YIG:Co and CaMnGe garnets serve rather as the model objects for demonstration of the mechanisms of polarization holographic recording. PC containing azobenzene dyes or azobenzene lateral groups presently are of interest due to perspectives of their use as optically active mediums, in particular as polarization sensitive mediums. We present results of investigation of the electrooptical and information properties of polymeric films containing azobenzene fragments as well as the films of polycomplexes of these fragments with cobalt.

The physical nature of photoinduced effects (PIE) in garnets is connected with the formation of optical or/and magnetic anisotropy within the illuminated sample region showing itself in the experimentally observed photoinduced linear birefringence or a spin reorientation transition. In the polymeric compositions containing azobenzene polycomplexes photoinduced optical anisotropy appears under influence of polarized light which is absorbed by the azobenzene groups and causes changes of isomeric structure.

DESIGN OF THE DYE-SENSITIZED SOLAR CELL

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A dye-sensitized solar cell (DSSC) is a low-cost solar cell belonging to the group of thin film solar cells. It is based on a semiconductor formed between a photo-sensitized anode and an electrolyte, a photoelectrochemical system.

Because it is made of low-cost materials and does not require elaborate apparatus to manufacture, this cell is technically attractive. Likewise, manufacture can be significantly less expensive than older solid-state cell designs. It can also be engineered into flexible sheets and is mechanically robust, requiring no protection from minor events like hail or tree strikes. Although its conversion efficiency is less than the best thin-film cells, in theory its price/performance ratio (kWh/(m2·annum·dollar)) should be high enough to allow them to compete with fossil fuel electrical generation by achieving grid parity.

DSSCs are currently the most efficient third-generation solar technology available. Other thin-film technologies are typically between 5% and 13%, and traditional low-cost commercial silicon panels operate between 12% and 15%. This makes DSSCs attractive as a replacement for existing technologies in "low density" applications like rooftop solar collectors, where the mechanical robustness and light weight of the glass-less collector is a major advantage. They may not be as attractive for large-scale deployments where higher-cost higher-efficiency cells are more viable, but even small increases in the DSSC conversion efficiency might make them suitable for some of these roles as well.

DSSCs degrade when exposed to ultraviolet radiation. The barrier layer may include UV stabilizers and/or UV absorbing luminescent chromophores (which emit at longer wavelengths) and antioxidants to protect and improve the efficiency of the cell. DSSCs degrade when exposed to ultraviolet radiation. The barrier layer may include UV stabilizers and/or UV absorbing luminescent chromophores (which emit at longer wavelengths) and antioxidants to protect and improve the efficiency of the cell.

We measured the transmission spectra of several organic dyes and tested different manufacturing techniques of DSSCs. Results of the experiments show promising methods chosen selection of dyes and design of DSSCs.

HETARYL DERIVATIVES OF 3-HYDROXYCHROMONE AS FLUORESCENT LIGANDS IN COMPLEXATION PROCESSES WITH METAL IONS

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Environmental monitoring is one of the most important activities of the efficient nature management. Great attention is attributed to the metal ions concentration control in the natural objects, and particularly in waters. 3-hydroxychromones (3HC) were described as highly sensitive fluorophores, responsing to the changes in their microenvironment parameters, including the presence and quantity of metal ions traces [1]. Complexation processes can occur between metal ions and 3HC, containing either aryl or heteroaromatic substituents in the position 2 of chromone ring [2]. The latter attract particular interest because of the possibility of participation in complexation processes, competing for metal ions with casual in the cromone family orthohydroxycarbonyl cavity. This can lead to the unusual effects, depending on the photophysical features of investigated molecules [3]. Our study of complexation of quinoline-, 2,5-diphenyloxazole- and benzimidazole derivatives of 3HC with different metal ions in solution and polymer films proved that spectral and fluorescent properties are closely tied with the way of metal ions binding. High affinity of diphenyloxazole derivative to the mercury ions (lg K = 7,9) resulting in the low detection limit of these species ($\sim 10^{-10}$ M) was discovered. It is well below the MPC for mercury in the drinking water. Complexation of quinoline-substituted 3HC followed by fluorescence ignition unusual for heavy metals complexes is discussed.

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[2]. Roshal A. D. et al., J. Phys. Chem. A, 102, 1998, 5907-5914.
[3]. Svechkarev D. et al., J. Phys. Chem. A, 2011 (in press)

ON OPTICAL PROPERTIES OF HOLOGRAPHIC SENSORS BASED ON SILVER EMULSIONS

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Holographic sensors (HS) based on silver emulsions targeted to analyze solution components give an interesting object in study of light scattering by an ensemble of nano-particles, since one can change the environment of the particles almost preserving their mutual location. Such a HS is a hydrogele polymeric matrix with thickness up to tens microns, which is fixed on a substrate. Optical properties of the HS vary in layers with the period of half wavelength of the recording light. The layers are almost parallel to the surface of the substrate. Thus, the holographic layer has a structure of the one-dimensional photonic crystal. Due to this structure, the hologram reflects the monochromatic light. Changing the period by the testing substation leads to changing the wavelength of the reflected light. A way to form such layers, the photographic one, is to create layers with different concentration of the nano-grains of silver or of silver compounds. Typical sizes of the grains are tens nm. The average distance between them is much less than the light wavelength. In these systems we realize a considerable change of the reflection coefficient with changing acidity of the solution. One of the reasons to study optical properties of these materials is to provide the proper work regime of the sensor. That means that the HS should work in the whole working range of concentrations as a thin photonic crystal. The hologram functioning is seriously influenced by the light scattering properties. In its turn, these depend on the type (metal or dielectric) and properties of the scattering center, and on its environment (mixture and ion concentration of the solution and of the hydrogele). The light scattering is the Raleigh one and can essentially limit the working range from the short wavelength side. Another important issue is to check the quality of the holographic layer, in particular, its homogeneity. To this purpose, we developed a colorimetric method of determination of the wavelength with the digital camera. On the other hand, one can check the emulsion homogeneity by the distribution of the light scattering parameters.

INFLUENCE OF OXYGEN IONIC IMPLANTATION ON THE OPTICAL AND ELECTRONIC PROPERTIES OF COBALT IN DIFFERENT STRUCTURAL STATE.

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Optical properties of cobalt, and also two-componental structures Co - O were explored in amorphous and crystalline by a method of states in a spectral interval (0,25- 17,0) μm (0,07 - 4,96 eV), on a non-standard spectroscopic ellipsometer.

Pure structures of Co - O are gained by method of magnetron sputteringon cooled by liquid helium leucosapphire substrates, the last are gained at addition in the vacuum chamber the 2 % of oxygen. From absorption spectrums $\sigma(h\nu)$ pure cobalt in amorphous and crystalline states and cobalt with oxygen impurities it is visible, (see fig.) that at the content of 2 % oxygen maximum at 0,18 eV moved on 0,09 eV.
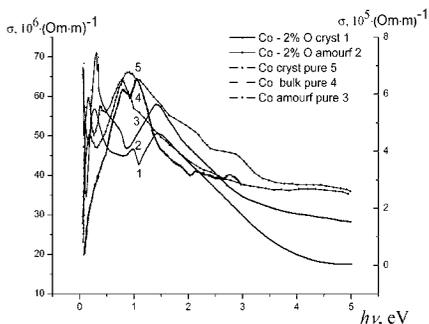
Fig. 1. Dispersion dependences of optical conductivity $\sigma(h\nu)$ pure to cobalt in crystalline (5) and amorphous (4) states, and also with the oxygen content in the chamber and accordingly 2 % (1) in the crystalline sample and accordingly in an amorphous state (2). Curves (3) and (4) correspond to pure amorphous cobalt and bulk cobalt.

The gauge at the left concerns pure cobalt, and on the right - to other samples.

The area of 0,7-1,2 eV fig. 1 (1) in a spectrum of crystalline structure Co - O (2 %) are shaped an absorption band with a maximum 0,97 eV, which

related with interband transitions of electrons from impurity bands on a Fermi level.

The uptake maximum nearby 1,44 eV is bound to a spectrum of pure cobalt but biased in area of high energies in a consequence disappear of vacancies and reduction of interatomic distances.

The long-wave strips in both spectrums for a crystalline and amorphous state too (fig. 1). The first maximum in a spectrum of an amorphous state of structure Co - O (2 %) at 0,31 eV conditioned formation of a new strip with big quantity of vacancies. The maximum in 0,35 eV in a spectrum of amorphous cobalt disappears, (fig. 1 (3)) i instead of it is shown the basic absorption band of cobalt 0,76 eV in the form of an inflexion Thus, in structure Co spectrum - 2 % O_2 are formed an impurity band, which is located a Fermi level, and also an additional band, which relating to vacancies.

HOLOGRAPHIC SENSORS

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Holographic sensors based on the hydrogel containing affinity groups sensitive to certain components of gaseous and liquid mixtures are perspective class of sensors. The sensor reflects a light in the same wavelength which was used for a hologram preparation. After the contact with an analyte, the analyte sensitive matrix changes its configuration, and the distances between layers of silver in the hologram are changed. As a result, the wavelength of a reflected light also changes. It is desirable that these changes were in the visible range (400-780 nm).

The photosensitized silver halogen nanocrystals were synthesized in the hydrogel matrix, the matrix was immersed in water and irradiated by the red He-Ne laser (632,8 nm, power - 15 mW)[1,2] or Blue violet laser pointer (405 nm, 10 mW), Blue laser pointer (473 nm, 10 mW), Green laser pointer (532 nm, 30 mW)

The matrix consisted of three-dimensional polymer net (N,N'-methylene-bis-acrylamide (bis) as crosslinking agent) based on the copolymers of acrylamide (AA), N-acryloyl-3-aminophenylboronic acid (AMPh) and additive as acrylic acid (AK), N-ε-methacryloyl-lysin (Lys), 2-(dimethylamino) ethylmethacrylate (DMA). Differences in the replay of these sensors correspond to pK of components in polymeric matrices, when the charge appears (or disappers) and matricies swelling takes place.

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[2]. А.В. Крайский, В.А. Постников и др., Квантовая электроника, 40 (2) 178-82 (2010)

INVESTIGATION OF CHANNELS OF CS-137 AND K TRANSFER FROM SOIL TO PLANT UNDER NATURAL CONDITIONS WITH OPTICAL AND GAMMA SPECTROMETRY

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To predict cesium concentration at the plant under natural conditions we must determine conditions for prevailing of low-affinity and high-affinity channels of cesium and potassium transfer to the plant under natural conditions at different cases. The aim of this work - to investigate cross points of prevailing of low-affinity or high-affinity channels of transfer of cesium and potassium to plant under natural conditions.

We investigated dependence of plant ^{137}Cs uptake on content of the soil solution and on the soil humidity. We carried out our investigations at field conditions and investigated growing at experimental sites with different types of soil different plants during two seasons (2002 and 2003 years). The lands are situated in 30 km from Chornobyl Nuclear Power Plant in the Northeastern direction. There were three types of soil: land A – based on glacial-water sand, soddy-podzol, middle podzol silts and soil; land B – based on decomposed middle thick sedge, rush and wood peat low-lying type peat soil; land C – based on glacial-water sand loam, soddy-podzol middle podzol sandy loam with signs of temporal excess humidification soil.

We sowed, mixed together, at these sites, fast-ripening plants that are as divergent from each other as possible. The roots of the plants are adjacent in the soil and were sowed several times during each season. We harvested samples several times. Every time we sampled, we took samples of soils, samples of the sowed plants, (if they had grown), and samples of wild plants. The conditions for all plants were the same, since they were growing together at the same land at the same time.

The soil solution was extracted from the soil using the centrifuge. We determined ^{137}Cs content in plants and in soil solutions with gamma-spectrometer and chemical content of plants and soil solutions with optical method with ICP spectrometer.

There are many channels of potassium transition to plants. We can't

identify them on the basis of our data. But we can distinct, if it is high- or low-affinity channel at the every case.

Data of our experiments show that sometimes potassium transfer via high-affinity channel is prevailing at rather high potassium concentration at the soil solution (but soil humidity is small), and sometime potassium transfer via low-affinity channel is prevailing at rather low potassium concentration at the soil solution (but soil humidity is high). We suggested explanation of this phenomenon. Prevailing of low-or high-affinity channel of potassium transfer is determined by needs of the plant in potassium. If transferred via low-affinity channel potassium is not sufficient for the plant, the plant uptake potassium via high-affinity channel, too.

We can conclude from our data that for all the investigated experimental sites, kind of plants and time caesium transfer to the plants via low-affinity channel.

POLARIZED STATIC FOURIER-SPECTROMETER

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This paper considers the principle of a static Fourier spectrometer (SFS) of polarization type (PT) own designed spectrometer and its advantages over other spectrometers. The phase difference between interfering beams of the described device is formed by the rigid crystals of optical system, which ensures its stability during operation in high vibration conditions. Device is designed as a compact monoblock, which also improves the reliability of measurements. The volume of the spectral device is smaller than a tennis ball. Significant area of localization of interference pattern allows direct measurement of the intensity of the interference pattern without use of optics, which reduces the size and simplifies the measurement process. Speed of measurements is limited by the time of registration of CCD («Charge-Coupled Device»). Features of the data processing, which is based on a theorem of scaling the Fourier transform, allows "free" positioning of CCD - matrix relative to the SFS. Furthermore SFS PT has one important advantage over other SFS - the ability to measure polarization characteristics of radiation. The device tested by measuring the emission spectra of white LEDs. Inverse Fourier transform of the detected spectrum agrees well with the spectrum obtained by the "usual" method.

LASER STIMULATED DESORPTION OF METHANE OF COAL SAMPLES

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The study of methane content in coal-beds and its desorption is very important practical task. The data on the methane supplies in coal is used for estimation of explosion risks in mines, potential of methane supplies as sources of natural gas and estimation of methane impact into the local or global environment pollution and greenhouse effect.

The methane desorption from the coal substance both by filtration and solid-state diffusion is the subject of many studies [see, for example 1]. The variety of desorption mechanisms needs the various techniques of its study. We discuss the application of laser stimulated desorption of methane by coal samples and laser absorption spectroscopy detection and concentration in atmosphere measurement.

The methane laser desorption has been studied in sealed glass cell having optical windows for laser radiation, both pulsed powerful infrared radiation for stimulation of desorption process and infrared CW radiation for methane absorption measurement.

The laser action onto the methane-contained coal samples stimulates a number of methane-desorption processes: methane filtration due to laser destruction of pore walls and heating of samples, thermal activation of solid state diffusion, surface desorption of methane absorbed by coal surface etc.

The methane desorption stimulation in the samples irradiated by infrared nanosecond, picosecond and femtosecond laser pulses was studied and possible machanisms of laser of stimulation samples heating and stimulation of methane diffusion, includingna thermal desorption of methane was studied laser sources used in experiments of methane content in experimental phstudy Under the proposed model of mass transfer of methane to construct asymptotic for large and small times, expressing the time dependence of gas concentration, and a comparison of experimental data with results of numerical calculation A number of methane sensors are designed for methane detections in atmosphere of some sa, for eThe one-page (page size A5) abstract should be written in English in accordance with this sample.

[1]. Alexeev A. D. Methane desorption from a coal-bed / A. D. Alexeev, E. P. Feldman, T. A. Vasilenko // Fuel. – 2007. – Vol. 88, N. 16. – P. 2574 – 2580

SPECTRAL PROPERTIES OF LEDS BASED LIGHT SOURCE FOR APPLICATION IN MUSHROOM CULTIVATION

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It has been proven that light is important morphogenetic factors for growth and development of many cultivated mushrooms. It has been shown that light with wavelengths of 650 nm and 530 nm has essential influence on the growth regulators and activity on growth processes of these mushrooms and has modified the lipid and carbohydrate spore composition. The light-induced modifications had prolonged action and were transmitted to the following ontogenetic stages, from spores to mycelium. Infrared rays in definite doses cause the intensification of growth in culture of medicinal mushrooms Coriolus vaporarius (Pers.:Fr.) Bond, et Singer and Serpula lacrimans(Wulf. apud. Jacq.:Fr.) Schroet. The absence or existence of light influence during the period of vegetative mycelial growth affects the character of further bearing [1].

The LED-based illumination with a proper proportion of light components enhances photosynthetic productivity and ensures better plant morphology in comparison with illumination using high pressure sodium lamps High-power AlInGaP-based red LEDs emitting at wavelengths as close as possible to 660nm as well as further development of LEDs emitting in the vicinity of 640nm are of major interest for horticulture applications. [2].

The mushroom cultivation needs the light environment with rather different spectrum and intensitycomparing with plants cultivation. Here we present the photobiology light source based on the light emitting solid state diodes (LED) for applications in Greenhouse Environment. Basing onto the previous investigations, we designed and prepared the illuminating system with ability of tailoring of output light spectrum. The composition of blue and red parts of light spectrum can be adjusted depending of experimental needs.

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[2]. N. Pojedinok, A. Buchalo et al. The Light Factor in Biotechnology Cultivation of Medicinal Mushrooms International/ Journal for medicinal mushrooms, v. 7, no 3, (2005).

DYNAMICS OF Q-SWITCHED DIODE PUMPED SOLID STATE LASER WITH DYE-DOPED POLYMER MODULATOR

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The development of polymer-based laser elements for tunable solid-state organic dye lasers, Q-switch modulators for flash lamp and diode pumped solid state lasers is very attractive due to ability of substitution of the expensive crystal-based elements by cheap polymer ones and wide modification of laser elements properties. The solid-state dye laser with dye-doped polymer elements have the advantage compared to liquid dye lasers being free of solvent handling, having a small size, and being easy to operate. During the past few decades, these laser elements are the subjects of considerable interest and research activity. Special object of interests is the photostability of organic dye molecules trapped in transparent polymer matrices. The old problem of photochemical bleaching of dyes by light, well known in textile industry, is a problem for laser application too. The bleaching mechanism is not well understood, and it may well vary from one class of dyes to another.

The stability of dyes molecules can be varied depending on the chemical and physical properties of dye molecules and polymer matrices.

The photochemical bleaching of solutions of organic dyes (rhodamine, astroflacksynes) in polymer matrices based on polyurethane and polyurethane acrylate was studied. The strong grows of laser dyes photostabity in polyurethane matrices comparing with polyurethane acrylat one is demonstrated.

The polymer based dye-doped Q-switch modulators were tested in diode pumped solid state lasers. The dynamic of laser generation was studied at wide range of operational parameters and effective and stable operation of polymer modulators was demonstrated.

LUNAR PHASES IN THE VARIATIONS OF [214]PB AND [214]BI CONCENTRATIONS IN AIR OF UNIVERSITY BUILDING

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Aerosols of radioactive [214]Pb and [214]Bi can get into the human body during respiration. In the air they are produced by [226]Rn decay. Inhalation of Radon and its decay products increases the risk of c ancer. The concentration of these isotopes in the air of university building is the subject of our research. Because the Radon source is [238]U, which is scattered in the soil, monthly variation in the gravitational perturbations of the earth's crust can affect the Radon' and its decay products'concentrations.
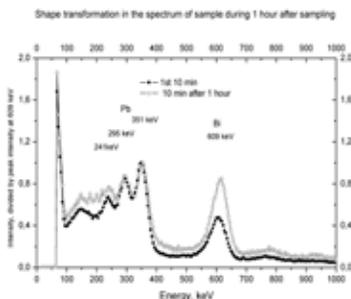
To determine the concentration of Pb and Bi we pumped over the air through the filter, which is besieged by a 90-95% of these atoms. One sample corresponded to the air volume approximately 10 cubic meters, pumping speed - 1 kub.meter / min. Identification and concentration measurement of these atoms were performed using K-lines in the spectra of spontaneous luminescence and nuclear transitions 351 keV, half-life time of the excited state is 26.8 min (Pb), and 609 keV (19 min, Bi). Emission spectra recorded by NaI-Tl detector 80x80 mm, followed by 1024-channel amplitude analyzer. The spectrum of sample after pumping air was compared with the spectrum of activated carbon, which 3 days were placed in the room under study. Also variations in the spectrum of air in the chamber of detector, and changes in the spectrum of the sample during two hours after sampling where controlled. Revealed that the [214]Pb and [214]Bi concentrations correlate with the phases of moon indeed, which may indicate the combined influence of solar and lunar tidal cycles in the Earth's crust. The ratio of maximum to minimum concentrations is 2,5-3 times.

9
COMPUTER SIMULATION

QUANTUM-CHEMICAL INTERPRETATION OF THE IR VIBRATIONAL SPECTRA OF 2-AMINOPURINE WITH CYTOSINE AND THYMINE

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2-aminopurine (2AmPur) is a purine derivate comparable to adenine (Ade) and guanine (Gua), its chemical structure differs from Ade (6-aminopurine) only in the position of the amino group NH2. 2AmPur is known to be a strong mutagen.

Literature data on vibrational spectra investigations (as theoretical, so experimental) of 2AmPur (neutral or protonated at N1 atom) and its H-bonded complexes with cytosine (Cyt) or thymine (Thy) are not available hitherto, although vibrational spectroscopy is one of the most perfect tools for studying the properties of the hydrogen bonds.

The aim of this work was to determine the characteristic features of the effect of hydrogen bonds formation on the IR vibrational spectra of complementary base pairs compared with the vibrational spectra of the nucleic acid bases using quantum-chemical calculations.

Using theoretical study on the B3LYP/6-311++G(d,p) level of theory we have compared vibrational spectra of 2AmPur (neutral or protonated at N1 atom species) with Ade and H-bonded complexes of 2AmPur (neutral or protoned at N1 atom species) paired with Cyt or Thy with Ade·Cyt and Ade·Thy base pairs.

We established that discrepancies in the spectra as monomers so base pairs are located in the high-frequency region. Namely, we can distinguish spectra of the Ade, 2AmPur from the spectra of Ade·Thy and 2AmPur·Thy accordingly by the position of the symmetric stretching vibrations of the NH2 group of purine, while spectra of Ade, 2AmPur, 2AmPur$^+$ and Ade·Cyt, 2AmPur·Cyt and 2AmPur$^+$·Cyt are indistinguishable by this band as far as by $\nu(NH_2^{anti})$ and $\nu(N9H)$ stretching modes of purines accordingly due to the close location of the $\nu(NH_2^{sym})$, $\nu(NH_2^{asym})$ and $\nu(N9H)$ stretching modes. For base pair intense bands corresponding to the vibrational stretching frequencies of the exocyclic groups are observed.

Differences in the IR spectra of isolated bases and base pairs besides of the aforementioned modes consist in the distinctions of the location of the most intense bands – for monomers the most intense bands are situated in the low- or middle-frequency region and correspond to the out-of-plane or scissors vibrations respectively, while for the base pairs the most intense bands are located mainly in the high-frequency region and corresponds to the stretching vibrations of the exocyclic groups.

THE ANALYSIS OF THE MATRIX TYPE INFLUENCE ON THE INNER ROTATION BARRIERS HEIGHT AND THE TORSION STATES SPLITTING OF THE METHANOL MOLECULE IN THE GROUND VIBRATIONAL STATE

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Matrix isolation of the studied molecules at low temperatures is a very effective method for the investigations of their structure and spectral characteristics. It is generally accepted that the matrix consisting of inert gas atoms isolates the individual molecules of the studied substance and have no influence on their structure and spectral properties. But the recent experimental studies [1-3] have shown that there is the interaction between Ne atoms and the studied molecules, determining the splitting of the absorption bands in FTIR spectra of methanol in these matrices at 2.7 – 7 K [1]. The idea of the work is that though the neon matrix influence on the molecule excludes its free rotation as a whole, the torsion tunneling is still possible. As a result, the ground vibrational state is split in more energetically favourable torsion-vibrational state of A_1 type and the slightly higher analogous state of E type. As it is indicated in [4] the energy difference between these stated in the gas phase is 9.12 cm^{-1}. Due to the interaction with the matrix the potential barriers heights increase and the corresponding difference decrease to 6.7±0.5 cm^{-1}.

The excited vibrational states of methanol are also split due to the torsion-vibrational interaction, but the value of the splitting changes at the transition from one fundamental state to another. According to [2] for the definite fundamental vibration at the transition from the ground state to the excited one the splitting value usually decreases, for some transitions it remains constant, and in the case of the deformation vibration of the hydroxyl group it essentially increases (20 cm^{-1}). The matrix influence also causes the breaking of the selection rules $A_1 \rightarrow A_2$ and $E \rightarrow E$, which are strictly fulfilled for the gas phase, and the transitions $A_1 \rightarrow E$ and $E \rightarrow A_1$ are presented in the matrix spectra with the intensities comparable with the intensities of the permitted ones. Note also the correlation between the symmetry of the excited fundamentals and the relative location of the torsion levels A_1 and E. For the vibrations of the methyl group generated by the E type in the assumption of C_{3V} symmetry, the torsion levels change their locations and the level of E type becomes lower, while for the rest of the vibrations the usual location of the torsion levels is typical, where the ground level is the one of A_1 type. It seems that more

natural and not requiring the idea of the torsion levels inversion is the consideration of these phenomena in terms of the general torsion-vibrational levels. The ground vibrational state is totally symmetrical and hence the symmetry of the torsion-vibrational levels is determined by the symmetry of the torsion levels ($A_1 \times A_1 = A_1$ and $E \times A_1 = E$). It is so and for the excited torsion-vibrational levels connected to the totally symmetrical vibrations of the methyl group and other parts of the molecule. In the case of the excitation of the methyl group fundamentals, maintaining E symmetry, the symmetry of the ground torsion-vibrational level becomes $A_1 \times E = E$, while the excited torsion level of E type in combination with the vibrational state of the same type will contain the totally symmetrical component ($E \times E \in A_1$). As it is seen, the consideration of the general torsion-vibrational state changes the symmetry of the ground torsion-vibrational level at the excitation of the E vibrations. In the later work [5] the low-temperature FTIR spectra of methanol in nitrogen matrix are analyzed. It was noted that the interaction of methanol with this matrix is more essential. The increasing of the potential barriers of the inner rotation leads to fact that the splitting of the lowest torsion level in the ground and the excited states is close to zero, which, in its turn, causes the absence of the multiple structure of the absorption bands. In [5] it was noted that Ar in its matrix properties is closer to Ne.

For the theoretical estimation of the matrix influence on the heights of the potential barriers of methanol molecule the series of computer experiments was carried out. As the matrix material the Ar and Ne atoms as well as N_2 molecules were used. At the first stage the methanol molecules were surrounded by six gas atoms or molecules (X=Ar, Ne, N_2) and using the quantum-chemistry program [6] in the approximation B3LYP/cc–pVTZ the geometry optimization of the system methanol+matrix was carried out by all inner variables. At the next stage the space position of all six gas atoms or molecules was fixed and the dependence of the inner energy of methanol on the value of the torsion angle between hydroxyl and methyl groups in the interval from 0 to 60^0 with the step 10^0 was calculated. Simultaneously at each step the optimization of the methanol molecule geometry by the rest 11 inner parameters was carried out. The results of the calculations agree with the experimental data demonstrating the increasing of the potential barriers heights and, as a sequence, the decreasing of the value of the tunnel splitting of the torsional energy levels in the ground vibrational state in the series Ar, Ne, N_2.

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QUANTUM CHEMICAL CALCULATIONS OF ELECTRONIC SPECTRA OF BENZOXAZOLES UNDERGOING EXCITED STATE PROTON TRANSFER

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Excited state intramolecular proton transfer (ESIPT) as photoinduced enol-keto tautomerization has been studied for several decades both experimentally and theoretically to elucidate the microscopic reaction mechanisms. A number of the compounds that show ESIPT have also been probed as materials for a variety of applications such as laser dyes, UV stabilizers, plastic scintillators, emitting layers for OLED and media for non-linear optics.

Time-dependent density functional theory (TDDFT) calculations have been found to be a relevant tool for modeling spectral properties of dyes [1]. The TDDFT and approximate coupled cluster with single and double excitation (RICC2) methods have been applied to calculations of the electronic structure and potential energy surfaces of some substances undergoing ESIPT [2].

We have calculated the energies and oscillator strengths of vertical transitions for various rotameric and tautomeric species of benzoxazole derivatives that exhibit ESIPT (2-(2'-hydroxyphenyl)benzoxazole (HBO), 2,5-bis(2-benzoxazolyl) phenol (DBP) and 2,5-bis(2-benzoxazolyl)hydroquinone (BBHQ)) in the ground and first ($\pi\pi^*$) excited states with the use of the TDDFT and RICC2 methods for isolated molecules under assumption of the C_s symmetry. In the ground state the most stable structures are enol tautomers with OH…N hydrogen bonds. The number of molecules with OH…O hydrogen bonds is found to be small that accounts for the low intensity of the corresponding fluorescence bands of HBO and DBP. In the excited state of HBO molecule, the calculations yield stability of the keto tautomer by 0.18 eV in relation to the enol with a low barrier for the proton transfer (TDDFT) or the barrierless process (RICC2) so that the tautomer fluorescence is expected to predominate. In the case of DBP and BBHQ, the RICC2 results, predicting lower energies of keto structures in the excited state, are more consistent with the experimental findings. Nevertheless, TDDFT performs better in the calculations of the frequencies of the absorption and fluorescence bands.

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SIMULATIONS OF VIBRATIONAL SPECTRA FOR LARGE BIOMOLECULES

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Vibrational spectroscopy is a versatile, widely available and highly informative tool, which has been successfully used for conformational and structural studies of biomolecules and particularly nucleic acids for a few decades. In addition to the classical methods, namely infrared (IR) and Raman spectroscopy, recent development of the chiroptical vibrational techniques, such as vibrational circular dichroism (VCD) and Raman optical activity (ROA) significantly broadened the applicability of the vibrational spectroscopy and enhanced the obtained structural information.

However, due to complexity of vibrational spectra of biomolecules, large bandwidth, many overlapping vibrational bands and coupling of vibrations, clear and straightforward interpretation of the spectra is an ambiguous and tedious task. Theoretical simulations of the spectra can significantly simplify this task, providing unambiguous assignment of spectral features. Furthermore, they can additionally offer rich information on the system's energetics and interactions obtained from the first principles. Unfortunately, such simulations can be currently performed at necessary precision only for relatively small molecules, leaving biomolecules beyond the accessible molecular size.

A possible approach to partially overcome the molecular size limitation is Cartesian coordinate transfer (CCT) technique, which has been developed in our group [1]. The method allows to transfer molecular properties from smaller molecular fragments to larger systems, enabling one to compute vibrational spectra for relatively long oligomers of nucleic acids or peptides. The applicability of the CCT technique to compute IR and VCD spectra of various nucleic acid conformations will be demonstrated.

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THE INFLUENCE OF MOLECULAR CLUSTERIZATION ON VIBRATION SPECTRUM OF METHANOL

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The subject of research in this work is manifestation of intermolecular hydrogen bond in vibration spectrum. As subject of research was taken the simplest of alcohols- methanol. Urgency of work caused by the big role played by hydrogen bonding in structuring the most important for human fluids - water, natural physiological fluids, etc. Feasibility studies to select items based on the fact that methanol is the simplest one internal fluid molecular hydrogen bonds. Analysis of vibrational spectra of methanol, which contained molecules in crystalline argon matrix leads to the conclusion that with increasing temperature argon matrix increases the number of methanol molecules, which form cyclic clusters. In the frequency domain, where the apparent valency OH group vibrations can be observed vibrational bands associated with the dimer, trimmers, and tetrameter. Quantum-chemical simulation for methanol molecule and clusters up to tetramer were carried out. The calculations was based on the density functional theory in approximations of bi-exponential atomic basis 6-31G (d,p), the hybrid exchange three-parameter Becke potential and exchange-correlation Lee-Yang-Parr potential (B3LYP). The results of quantum chemical calculations of model spectra correlate with these findings. It is shown that intermolecular hydrogen bonding leads to changes of all vibrational spectra of methanol. In particular, undergo significant changes contour strips that related to valence vibrations of C-O bond. With increasing temperature argon matrix from 15 K to 50 K observed structures and expanding the disappearance of C-O vibrational bands. A similar result is fixed in frequency domain vibrational spectra of methanol, which manifested O-H valency vibration. In this temperature can be argued that in the matrix remain only four-and pyatymolekulyarni clusters. Methanol in the vibrational spectra of argon matrices at such temperatures similar to the spectra of liquid methanol. From this you can infer that in both cases were identical with the cluster structure.

DETERMINATION OF THE TYPE OF HYDROGEN BONDED FORMATIONS WHICH OCCUR IN HIGHER ALCOHOLS BY MEANS OF VIBRATIONAL SPECTROSCOPY AND QUANTUM-CHEMICAL MODEL CALCULATIONS

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The modern theory of liquids based on the fact that the structure and properties of real fluids is largely determined by structural features of nanoscale particles and the associative nature of the forces acting between them. It is known that these fluids are formed three-dimensional structure, consisting of several molecules related intermolecular hydrogen bonds - clusters. Special interest causes the system with intermolecular hydrogen bonds, which include alcohols. Alcohols are amazingly convenient object for studying hydrogen bonds. In contrast to more simple, but completely unchangeable molecules of water, alcohols can be "fit" under the necessary research by easy restructuring of the backbone to which the hydroxyl group attached [1].

The study of alcohol clusters conducted mainly for alcohol which molecules contain a small number of atoms: methanol, ethanol, n-butanol [2-4]. There are two basic topology of formation in alcohols structures which are connected by hydrogen bonds: formation of closed, cyclic clusters, when all hydroxyl groups in the structure involved in the creation of hydrogen bonds, and chain clusters, when one of the hydroxyl groups remain nonbonded on the "edge" of a cluster [1]. Theoretical calculations and experimental studies prefer the formation of cyclic clusters in the liquid phase [5]. However, similar cannot be say in the case of higher alcohols, because long alkyl groups may prevent molecules to form a compact structure.

In this work investigated such higher alcohols as heptanol and oktanol. Using the methods of quantum-chemical simulation we managed to establish possible structures arising from the molecules in the liquid phase and determine their energies and spectra. For reasons of energy utility of structures and comparing the calculated spectra with the experimentally obtained, it is determined the types of clusters that exist in this alcohols.

It is shown that although the energy, which accounts for one hydrogen bond, largest in the case of chain-like clusters, but the energy of the whole

formation more in the case of cyclic clusters. It is expected that there are cyclic clusters in the alcohols (of four molecules and more) with a small percentage of chain-like clusters which is the result that the spectral line intensity assigned to the vibration of the free hydroxyl groups decreases to the noise level. As evidence to the assumption this spectral bond practically not seen in the experimental spectrum.

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ONE-, TWO-, AND THREE- DIMENSIONAL POTENTIAL ENERGY SURFACES AND ANHARMONIC VIBRATIONAL FREQUENCIES FOR THE HCN-HF COMPLEX

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A nonempirical calculation of the HCN-HF complex to determine its geometrical parameters and frequencies was attempted. The electronic structure calculation of the complex was performed using the GAUSSIAN package of codes. In all the calculations we adopted the 6-311+G(2d,2p) basis. The electron correlation correction was accounted for by using the MP2 perturbation theory. The equilibrium configuration of the complex is linear with the atoms arranged as follows: HCN…HF. The equilibrium bond length r(HF) =0.9298 Å, the bond length r(CN) =1.1626 Å. For the equilibrium configuration, the electronic energy of the complex is -193.53787 au. The vibrational frequencies in the harmonic approximation were calculated. The values obtained are ν_1(H-F)=3897, ν_2(C-H)=3462, ν_3(C≡N)=2051, ν_4(N…H) =186, ν_5^1 (γ(HCN))=729, ν_6^1 (β(FHN))= 670, ν_7^1 (α(CNH))=83 cm^{-1}.

The possibility of calculating the vibrational frequencies of complex in the anharmonic approximation using the normal coordinates as the vibrational coordinates was analyzed. For all normal coordinates we computed the one-dimensional cuts of electronic energy of the complex, i.e., the potential energies of one-dimensional vibrations. The range of variation of each variable coordinate was wide enough to allow the description of the ground and several excited states of a one-dimensional anharmonic oscillator. The matrix elements of the potential energy operator were evaluated by Gauss–Hermite quadratures.

The anharmonic interactions between different vibrational degrees of freedom can be more important than the one-dimensional anharmonic corrections. Therefore, we considered all pairs of normal coordinates of the complex, calculated the two-dimensional potential energy surfaces using the GAUSSIAN package, and found the variational solutions of the two-dimensional vibrational Schrödinger equations in which the kinetic energy operator is the sum of the operators of the noninteracting harmonic oscillators.

For the large-amplitude librations the kinetic energy operators of HF and HCN molecules should be expressed in terms of their angular momenta. We obtained the variational solutions of nine one-dimensional and a number of two- and three- dimensional anharmonic problems. We calculated the nonempirical potential energy functions dependent on one, two, or three coordinates with the remaining coordinates fixed at their equilibrium values. In considering the librational motions, the Legendre polynomials were used as basis functions.

THE CALCULATION OF STRUCTURE AND IR SPECTRUM OF THE METHYL-B-D-GLUCOPYRANOSIDE BY DENSITY FUNCTIONAL METHOD WITH TACKING INTO ACCOUNT THE HYDROGEN BONDS FORMATION

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Theoretical research of IR spectrum and structure methyl-β-D-glucopyranoside tacking into account influence on them hydrogen bond realized in the sample have been conducted. By density functional method using B3LYP functional in basis 6-31 G(d) energies have been minimized and structures, electro-optical parameters, force constants, frequencies of normal modes in harmonic approximation and intensity in IR spectra of the elementary complexes with hydrogen bonds between methyl-β-D-glucopyranoside molecules presented by dimers have been calculated. The calculated spectra H-bond complexes have been compared with the calculated spectra of a separate molecule and with experimental spectra in a range of 400-3700cm^{-1}. Conclusions about structure of the sample methyl-β-D-glucopyranoside have been made and interpretation of it's IR spectrum have specified. Experimental IR spectrum of the sample is formed by spectra of different H-bond complexes.

STRUCTURE AND SPECTRAL CHARACTERISTICS OF ETHANOL MONOMER AND DIMER FROM THE DATA OF LOW-TEMPERATURE FTIR SPECTRA AND THE RESULTS OF NON-EMPIRICAL QUANTUM-CHEMICAL CALCULATIONS

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Ethanol is one of the simplest alcohols able to form cluster structures due to the hydrogen bonds formation. In comparison with methanol the number of publications devoted to the spectral-structure characteristics of ethanol is not so large [1, 2]. The dynamics of the C-O stretch vibration in ethanol in CCl_4 was investigated in [3], the calculations of the structure of some ethanol clusters in the approximations B3LYP/6-311G(d,p) and MP2/6-311+G(2df,2pd) are presented in [4, 5], IR spectra of ethanol and some heterodimers with the investigated molecule were obtained in [6]. Besides the typical as well for methanol possibility of the inner rotation around C-O bond in ethanol molecule there is the additional possibility of the inner rotation around C-C bond. Moreover, the investigated molecule can form some energetically non-equivalent conformers [4, 5]. These factors essentially complicate the vibrational spectrum of ethanol.

FTIR spectra of ethanol isolated in an Ar matrix were registered at different temperatures from 10 K to 50 K. The investigation of the ethanol monomer and dimer was carried out with quantum-chemistry program in the approximation B3LYP/cc-pVTZ. The calculations predict the existence of some conformers of both monomer and dimer. The analysis of the simulation results allowed to determine the conformation-sensitive spectral bands and to estimate the influence of the structure factors on the force constants.

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SIMULATION OF OPTICAL MODES IN CRYSTALLINE AND AMORPHOUS BINARY CHALCOGENIDES

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Novel applications of binary and multinary chalcogenide semiconductors during last decades in photonics, optoelectronics, sensorics motivate a steady interest to the search for the compositions with required properties. This work extends our previous studies (see, e.g., [1, 2]) and is intended to the deeper understanding of the optical and mechanical properties of complex chalcogenide compounds in bulk, film and nanosize forms. For the present optical modes studies we took as model materials the following extensively studied binary compounds ZnX, GeX_2, As_2X_3, Sb_2X_3, and Bi_2X_3, ($X = S$, Se, Te).

In this work, in terms of bond-orbital approximation developed by W. A. Harrison [3] we have calculated bond polarities, transverse and longitudinal optical modes, effective transverse charge, and dielectric permittivity for binary chalcogenides under investigation. In the calculations of the above-mentioned parameters for non-crystalline materials we took into account correlation between theoretical physical parameters and their experimental values (photoemission threshold, the band gap, transverse optical vibrational frequencies). Dependence of theoretic values of optical frequencies on the variations in possible bond length and valence angles in view of structural peculiarities of the investigated compounds has been analyzed. Vibrational frequencies were calculated both for heteropolar and homeopolar bonds. The results of calculation have been correlated with known experimental data determined from Raman spectra. Quantitative agreement between theoretical and experimental values for optical modes has been obtained.

Applicability of the proposed approach to the calculation of optical modes for multicomponent chalcogenide materials has been discussed.

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DESIGNING AN INTERFERENTIAL FILTER WORKING INA GIVEN SPECTRAL RANGE

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In this paper is analyzed the possibility to obtain an interferential filter for a given spectral range. Different filters were simulated for various layers of MBBA liquid crystal and rutile. Liquid crystals are complex, mesogene organic molecules which, under certain temperature conditions, present mechanical characteristics of a liquid (fluidity) and optical characteristics of a crystal (optical anisotropy) [1]. Rutile is one of the most common titanium minerals (TiO_2) which can contain in different amounts iron, nobium and tantalum [2]. It has among the highest refractive indices of any known mineral and exhibits high dispersion [2]. The majority of rutile crystals is transparent in the visible range and absorb in UV range [2].

The principal refractive indices of the samples were measured using Rayleigh interferometer. The main values of the refractive index were determined by means of the polarizer placed in the measuring beam having the transmission direction oriented parallel, respectively, perpendicularly, on the optical axis of the uniax substance [3- 5]. The simulation of the birefringence in the visible range was made in the basis of experimental data in order to determine Cauchy coefficients [4].

The aim of the study was to obtain filter with maximum of transmission factor at a given wavelength and with a minimal bandwidth. The changes induced by an external electric field both in the values of the main refractive indices and in birefringence determine modification for the light transmission factor of the considered device [5, 6].

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MINOR ACADEMY OF SCIENCES

Секція «Експериментальна фізика»

ДОСЛІДЖЕННЯ СТІЙКОСТІ КОНФІГУРАЦІЙ МАГНІТНИХ СИСТЕМ

Видро Роман Олегович

учень 9 класу комунального закладу "Харківський фізико-математичний ліцей № 27" Харківської міської ради Харківської області

У роботі здійснено дослідження стійкості різних магнітних систем. У процесі дослідження:

• проаналізовано теоретичні й експериментальні методи дослідження стійкості;

• використано методику візуалізації розподілу магнітного поля у просторі за допомогою залізної тирси;

• сконструйовано кілька варіантів експериментальних установок із використанням магнітних взаємодій;

• було проведено серію дослідів, отримано базу експериментальних даних;

• проведено аналіз експериментальних даних;

• на основі експериментів були сформульовані принципи побудови фізичної моделі та запропоновано саму модель;

• на основі моделі було отримано теоретичні пояснення явищ;

• зіставлення теоретичних і експериментальних результатів підтвердило їх узгодженість;

• обґрунтовано актуальність теми і можливість подальших досліджень.

ЕКСПЕРИМЕНТАЛЬНІ ДОСЛІДЖЕННЯ ЗАЛЕЖНОСТІ КОЕФІЦІЄНТУ ТЕРТЯ ВІД ТЕМПЕРАТУРИ

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Для проведення експерименту був виготовлений термостат, температура в якому забезпечувалася лампами розжарення. На дні установки міститься дерев'яна підставка під робочу поверхню і робоче тіло.

Коефіцієнт тертя визначався по вимірюванню прискорення досліджуваного тіла при горизонтальному русі. До тіла прикріплювалась нитка з тягарцем на іншому кінці, що була перекинута через блок.

Вимірювався час, за який тіло пройде певну відстань. При різних температурах проводилось по десять експериментів. Далі вираховувалися прискорення і коефіцієнт тертя. За результатами експериментів було встановлено, що коефіцієнт тертя має тенденцію до зменшення при збільшенні температури.

Були побудовані графіки залежностей коефіцієнтів тертя від температури і отримані такі температурні коефіцієнти: -0,0017 1/К для сталі об алюміній і – 0,0019 1/К для сталі об сталь. (Оксано, червоним виділив – це тире чи мінуси? Гугл толком не дає уявлення)

Можливою причиною цього є випаровування з поверхні металу молекул води, що «зліплюють» метали при ковзанні один по одному, тобто коефіцієнт тертя залежить від відносної вологості при даній температурі.

Далі було встановлено, що при сталій відносній вологості коефіцієнт тертя залишається майже сталим при різних температурах.

Отже, коефіцієнт тертя залежить від відносної вологості при даній температурі, причому він зростає при її збільшенні. У майбутньому планується провести більше дослідів для різних тіл і поверхонь та використовувати більш точні прилади для зменшення похибок.

ПРОГНОЗУВАННЯ ХАРАКТЕРИСТИК УЛЬТРАДИСПЕРСНИХ СУМІШЕЙ ЗА ДОПОМОГОЮ КОМП'ЮТЕРНОГО МОДЕЛЮВАННЯ

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Метою роботи є дослідження можливості визначення характеристик ультрадисперсних сумішей (зокрема молока) за допомогою експериментальних оптичних методів і комп'ютерного моделювання на основі явища розсіювання світла.

Основні завдання дослідження:

1. Експериментально дослідити розсіювання світла молоком різної жирності і з різною дисперсністю жирових часток.

2. Створити комп'ютерну двовимірну модель для дослідження проходження світлового променя через ансамбль сферичних жирових включень в однорідному середовищі (воді).

3. Дослідити можливості формулювання і розв'язання оберненої задачі, тобто можливості визначення жирності й дисперсності з експериментальних даних щодо розсіювання світла.

Дослідження засвідчило, що запропоновані у роботі прилад і комп'ютерна модель можуть бути альтернативним інструментами оцінювання системи, а можуть використовуватися комплексно. Для коректної роботи обох підходів на основі світлорозсіювання необхідно, щоб концентрація жиру та розміри жирових частинок були досить малими.

На основі результатів комп'ютерної симуляції продемонстровано, що жирність є не єдиним параметром, який визначає кутовий розподіл розсіяного світла, – не меншу роль відіграє і дисперсність жирових кульок. Уведені кількісні характеристики індикатриси розсіювання свідчать, що збільшення жирності за постійної диспергованості веде до збільшення відбивання світла при незмінному розсіюванні, а збільшення диспергованості при постійній жирності веде до майже ізотропного розсіювання світлового пучка.

ГУСТИНА МОЛОКА ЯК ПОКАЗНИК ЙОГО ЯКОСТІ

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Актуальність цієї теми полягає в тому, що понад 80% валового виробництва молока надходить на молокопереробні підприємства з особистих підсобних господарств населення, де умови його отримання і первинної обробки мають значні недоліки. Як правило, в таких господарствах застосовується ручне доїння, немає ефективних методів охолодження, на відміну від тих, що існують у колективних сільськогосподарських підприємствах (фермах), де здебільшого створюються оптимальні умови для виробництва молока з використанням відповідної доїльної та охолоджувальної техніки.

Незважаючи на те що до молока, яке заготовляється для молокопереробних підприємств, висуваються високі вимоги, досі залишаються недостатньо вивченими проблеми аналізу якості молока (зокрема його густини і наявності домішок у ньому, наприклад води чи солі) в домашніх умовах.

Метою пропонованої роботи є експериментальне визначення густини домашнього і магазинного молока у чистому вигляді та з домішками.

Предмет дослідження: густина промислового молока і молока, одержаного з особистих підсобних господарств населення.

Об'єктом дослідження є технологічний процес одержання молока з високим (стандартним) показником густини.

Матеріалом для дослідження були проби молока, які відбиралися в особистих підсобних господарствах Баранівського району, і молока марки «Селянське» виробництва ТОВ «Люстдорф», придбаного у супермаркеті.

Молоко – це колоїдний розчин жиру у воді, який містить також різні органічні та неорганічні сполуки. Хімічний склад молока становлять вода, сухі речовини (молочний жир, сухий знежирений молочний залишок) і гази (вуглекислий, азот, кисень, аміак).

Фізичні властивості молока: густина; в'язкість; поверхневий натяг; осмотичний тиск і t кристалізації; електропровідність.

Густина магазинного молока при різних температурах є дещо вищою, ніж густина домашнього молока. Однак зазначені зразки мають різний коефіцієнт об'ємного розширення: для магазинного молока він

менший і наближається до коефіцієнта об'ємного розширення води. Це підтверджує той факт, що магазинне молоко – розчин хімічних елементів у воді. Отже, вміст домішок у молоці впливає на зміну його коефіцієнта об'ємного розширення.

Відношення густини молока та його розчинів до температури має лінійний характер і виявляє обернено пропорційну залежність: чим вища температура – тим менша густина.

Користуючись наведеними методами дослідження, у домашніх умовах за певної температури можна визначити густину молока, наявність і кількість води у ньому. Однак аналіз на вміст рідини приблизно однакової густини в молоці є не досить досконалим і точного визначення не дає, тому потрібні інші види досліджень, наприклад хімічний аналіз.

ДЗИГИ ДИВНИХ ФОРМ: ВІД ТЕОРІЇ ДО ПРАКТИКИ

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Багатьом дітям і дорослим відома іграшка, яка називається дзигою. Дзига, що швидко обертається, може слугувати не лише потішною іграшкою, а й прекрасним демонстраційним приладом при вивченні законів динаміки обертального руху твердого тіла. Дзиги, які продають у відділах іграшок магазинів, мають форму виключно тіл обертання. А чи обов'язковим є таке обмеження на форму? Чи можна зробити дзигу якої-небудь незвичайної форми, але щоб вона оберталася не гірше за куплену в магазині? Наші попередні дослідження привели нас до позитивної відповіді.

Тому мета оригінальної частини нашого дослідження полягала в тому, щоб теоретично обґрунтовано запропонувати нові форми дзиг, які б не були тілами обертання. Зразки таких дзиг могли б служити демонстраційними приладами для кращого засвоєння студентами і школярами окремих важливих питань динаміки обертального руху твердого тіла.

Актуальність постановки заявленої мети стає очевидною після критичного аналізу тих навчальних посібників, що з'явилися останнім часом в Україні: він засвідчив, що динаміка обертального руху твердого тіла є непростою темою не лише для школярів і студентів, а й для авторів деяких підручників.

У результаті роботи з навчальною літературою і виконання завдань, що містяться в посібнику для самостійного ознайомлення з поняттями тензора і еліпсоїда інерції, були зроблені теоретичні висновки, важливі для конструювання дзиг незвичайної форми. На підставі цих висновків були створені декілька експериментальних зразків дзиг, що явно відрізняються за своїми формами від тіл з віссю матеріальної симетрії. Ці зразки успішно пройшли експериментальну перевірку.

ДОСЛІДЖЕННЯ ФАЗОВИХ ТРАНСПОРАНТІВ ДЛЯ ГЕНЕРАЦІЇ ОПТИЧНИХ ВИХОРІВ

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У роботі розглянуті теорія і методика отримання та дослідження комп'ютерно синтезованих транспарантів. Фазові транспаранти – це класичний метод для отримання гвинтових дислокацій (оптичних вихорів). Оптичні вихори – новий тип хвильових полів – розглядаються в сучасній оптиці і є особливим поширенням електромагнітного поля, у якого амплітуда (інтенсивність) дорівнює нулю, а фаза є невизначеною і відчуває стрибок. Хвильовий фронт оптичного вихору – це гелікоїди (наприклад гвинт). Кількість гілок гелікоїда називається топологічним зарядом такого вихору.

Визначено кути дифракції, а також крок дифракційних елементів. На інтерферометрі Маха-Цендра були ідентифіковані оптичні вихори з різними топологічними зарядами. Показано можливості практичного застосування отриманих оптичних вихорів. У процесі роботи порівняно якість транспарантів з використанням фотонаборочного автомата і класичний метод з використанням фотоплівки (Мікрата).

Вихрові пучки з кільцевою формою можуть використовуватися в лазерній технології обробки матеріалів, у процесі створення активного елементу лазерів, лазерного пінцета.

СТРИБАЮЧЕ ПОЛУМ'Я

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В основі умови дослідження – задача XIX Всеукраїнського турніру юних фізиків 2010/2011 навчального року.

Вивчалась поведінка полум'я свічки між двома зарядженими паралельними пластинами (така система є плоским конденсатором).

Поведінка заряджених частинок усередині такої системи визначається наявністю і характеристиками електричного поля.

Отже, для з'ясування питання, поставленого в задачі, слід вивчати поведінку полум'я залежно від:

- напруги на конденсаторі при сталій відстані між обкладками;
- відстані між обкладками при сталій напрузі.

Джерелом високої напруги (25 кВ) був електронний перетворювач "Розряд-1", у якого величина вихідної напруги лінійно залежить від напруги живлення приладу.

Усі етапи експерименту фіксувалися фото- та відеозйомкою. Внаслідок того, що при пробої картина суттєво спотворювалася, критичні значення напруженості поля свідомо не досягалися.

Кут відхилення полум'я в електричному полі пов'язаний із напруженістю електричного поля. При певних напруженостях поля у полум'ї «народжуються» негативні іони.

КУЛЬОВА БЛИСКАВКА ЯК ФІЗИЧНЕ ЯВИЩЕ

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У вступі висвітлюються завдання роботи, дається визначення кульової блискавки та запитання, які вона ставить. Робота описує властивості цього явища, гіпотези про природу та джерела енергії кульової блискавки, досліди вчених з відтворення її, докладніше розглянуто плазмову гіпотезу як найбільш імовірну з точки зору автора.

Робота створена так, щоб повно і водночас лаконічно описати аналіз результатів спостережень кульової блискавки, на основі якого зроблено аналітичні дослідження гіпотез, що намагаються пояснити виникнення цього явища.

Висновки викладено аргументовано, стисло і відповідно до змісту роботи. Робота доводить актуальність цієї теми у багатьох галузях.

ПРОСТИЙ ШУКАЧ ПРИХОВАНОЇ ЕЛЕКТРОПРОВОДКИ

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Нині електрика займає провідне місце в побуті та промисловості. Більшість приладів працюють на електриці. Пошук силових кабелів підведення електроструму, як у домашніх, так і у виробничих приміщеннях, є одною з важливих проблем у повсякденному житті. Електромережа є джерелом електромагнітних хвиль.

Мета роботи: винайти і сконструювати найпростіший прилад для пошуку прихованої електропроводки.

Електромагнітне поле – це поле, яке описує електромагнітну взаємодію між фізичними тілами і створюється зарядами. Непорушні заряди створюють електричне поле, рухомі заряди — електричне й магнітне поля. Електромагнітне поле, яке породжується зарядами й струмами, діє на заряди і струми у фізичних тілах. Електромагнітне поле може виконувати роботу з переміщення зарядів й обертання магнітних моментів, а оже має потенціальну енергію. Електромагнітне поле, створене зарядами, поширюється у просторі у вигляді електромагнітних хвиль. Отже, взаємодія заряджених тіл не є миттєвою. Зміна положення одного заряду викликає зміну сили, з якою він діє на інший заряд, лише через проміжок часу, потрібний для того, щоб електромагнітна хвиля подолала відстань між зарядами.

На сьогодні існує велика кількість приладів, які фіксують електромагнітне випромінювання. Вони мають певні переваги, але водночас і суттєві недоліки, зокрема високу вартість. Запропонований розроблений прилад, на нашу думку, є оптимальним розв'язанням проблеми. У порівнянні із прототипами розроблений прилад недорогий, простий у використанні, ефективний при пошуку прихованої електропроводки.

Спочатку прилад був зібраний на вітчизняних транзисторах і резисторах. Проте оскільки їх немає у продажу, прилад був переведений на імпортні транзистори і резистори, що дало змогу покращити якість звукового сигналу, який видає динамік. У подальшій розробці прилад буде переведений на сучасні SMD-компоненти (від surface mounted device — прилад, що монтується на поверхню) і дискові батарейки. Це дасть змогу мінімізувати розміри приладу і помістити його в корпус із кулькової ручки або лазерної указки.

Прилад одразу здобув популярність у нашій школі. Їм зацікавились учителі – для пошуку прихованої електропроводки у власній оселі.

ДОСЛІДЖЕННЯ ЗАЛЕЖНОСТІ ШВИДКОСТІ ОХОЛОДЖЕННЯ ТІЛ ВІД КОЛЬОРУ Й МАТЕРІАЛУ

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У природі передавання теплоти від одних тіл іншим може відбуватися по-різному. Розрізняють три види теплообміну: теплопровідність, конвекція, теплове випромінювання.

Метою нашої роботи було дослідження залежності швидкості охолодження тіл від їх кольору і матеріалу.

Під час виконання експериментів були проведені дослідження залежності швидкості охолодження тіл від матеріалу, з якого вони виготовлені, та їх кольору, побудовані графіки, що підтверджують правильність отриманих результатів.

З метою зменшення випадкової похибки для кожного зразка було проведено три серії експериментів, обчислено похибку вимірювань, загальну похибку виконаних досліджень.

За результатами отриманих експериментальних даних можна зробити такі висновки:

1. Найшвидше охолоджується до кімнатної температури (20 °C) тіло, виготовлене з міді, найдовше охолоджується тіло, виготовлене зі свинцю.

2. Швидкість охолодження тіл залежить від матеріалу, з якого вони виготовлені, тобто від його фізичних і хімічних характеристик.

3. Швидкість охолодження тіл залежить від кольору тіла.

За однакових умов найшвидше охолоджується чорне тіло (92,24064 Дж/с), найдовше – тіло, пофарбоване у білий колір (82,20269 Дж/с). Нефарбоване тіло (природний колір алюмінію – сірого спектру випромінювання) має швидкість охолодження 88,1712 Дж/с.

Результати досліджень необхідно враховувати при фарбуванні тіл, що сприятиме запобіганню зайвих втрат енергії.

Секція «Теоретична фізика»

МОДЕЛЮВАННЯ І ВІЗУАЛІЗАЦІЯ РУХУ ВИХРОВОГО СЛІДУ ЗА ПОВІТРЯНИМ СУДНОМ

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Для моделювання і вивчення вихрових слідів літаків використовують різноманітні методи теоретичних досліджень: пряме числове моделювання турбулентного руху на базі рівнянь Нав'є-Стокса, моделювання великих вихорів з використанням управлінь Нав'є-Стокса і підсіткової моделі турбулентності, а також числове розв'язання рівнянь Рейнольда. У роботах С. М. Білоцерківського було запропоновано використовувати метод дискретних вихорів (МДВ) для моделювання вихрового сліду літака.

Кожен із методів знайшов застосування в моделях спутного сліду. Ці моделі створювалися для розв'язання чотирьох основних завдань: завдання літака-генератора сліду, взаємодії наступного літака з вихором від попереднього, моделювання турбулентної атмосфери і руйнування вихрового сліду.

У роботі розглянуто розв'язання проблеми візуалізації спутного сліду від літака генератора, щоб диспетчер повітряного руху міг повністю отримувати загальну картину в повітряному просторі і видавати команди, що відповідають метеорологічним даним.

ВИЗНАЧЕННЯ МЕХАНІЧНИХ ХАРАКТЕРИСТИК ЗА ДОПОМОГОЮ МІКРОТВЕРДОСТІ

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У роботі досліджували модуль нормальної пружності E (модуль Юнга) і межу пропорційності за допомогою мікротвердості. Мікротвердість вимірювали приладом ПМТ-3. Для дослідження вибрали дисперсійно-твердіючі сплави (ДТС) Al-4%Cu і Al-2%Cu, які широко використовуються в народному господарстві.

Дослідженнями продемонстровано, що можливе визначення E за формулою Герца:

$$d^3 = 6PR\left(\frac{1-\mu_1^2}{E_1} + \frac{1-\mu^2}{E}\right)$$

Звідки можна знайти

$$E = \frac{1-\mu^2}{\frac{d^3}{P}\frac{1}{6R} - \frac{1-\mu_{\text{и}}^2}{E_{\text{и}}}}E = \frac{1-\mu^2}{\frac{d^3}{P}\frac{1}{6R} - \frac{1-\mu_{\text{и}}^2}{E_{\text{и}}}}.$$

Отже, при відомих μ, $\mu_{\text{и}}$, $E_{\text{и}}$, R для визначення E необхідно виміряти величину, діючу на індентор навантаження P і відповідне їй значення діаметра контакту d.

Методика визначеня межі пропорційності (пружності) за результатами втискування індентора в плоску поверхню, основою якої є різні показники степеня в залежностях між діаметром відбитку d і навантаженням P у пружній і пластичних ділянках, описується рівняннями Герца і Майєра:

$$P = \frac{1}{3D\left(\frac{1-\mu^2}{E} + \frac{1-\mu_1^2}{E}\right)}d^3, \qquad P = ad^n,$$

де E, E1, μ, μ_1 — модулі нормальної пружності та коефіцієнти Пуассона індентора і випробовуваного матеріалу; a, n — константи пластичності, причому n має значення, близьке до двох.

Розходження між E, визначеними вдавлюванням та іншими способами, перебуває для більшості випробуваних матеріалів у межах 3%.

Межі пропорційності $\boldsymbol{\sigma}_{\text{ПЩ}}$ (Мпа), визначені методом втискування і розтягу для алюмінієвих сплавів|

Отже, дослідження свідчать про можливість широкого застосування методу мікротвердості для отримання не тільки стандартних, а й спеціальних механічних характеристик. Це дає змогу виміряти механічні властивости деталей без їх пошкодження.

ПЕРШИЙ ТА ДРУГИЙ ЗВУКИ У НАДПЛИННОМУ ГЕЛІЇ ТА БОЗЕ-АЙНШТАЙНІВСЬКОМУ КОНДЕНСАТІ

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Робота присвячена теоретичному розрахунку швидкості поширення першого і другого звуків у таких вироджених квантових системах, як надплинний гелій і розріджений бозе-газ за наявності конденсату. Зацікавленість до дослідження таких систем викликана їх специфічними властивостями. Зокрема, у вищезгаданих системах квантові ефекти проявляються на макроскопічному рівні.

Мета роботи полягає у відтворенні схеми опису першого і другого звуку для надплинного гелію-4 на основі лінеаризованих рівнянь дворідинної гідродинаміки і застосуванні цієї схеми до досліджень звукових мод в атомарному бозе-газі за наявності конденсату.

У роботі якісно проаналізовано умови утворення бозе-айнштайнівського конденсату в розрідженому атомарному газі.

Використовуючи схему досліджень, розвинуту для гелію-4, отримано вирази для швидкостей першого та другого звуків, які можуть поширюватися у розрідженому атомарному бозе-газі за наявності конденсату.

Проведено порівняльний аналіз звуків у надплинному гелії-4 й атомарному бозе-газі за наявності конденсату. Зокрема, засвідчено, що колективні моди в атомарному конденсованому бозе-газі мають основні характерні особливості, притаманні першому та другому звукові в 4He-II. На відміну від 4He-II, у якому другий звук поширюється у вигляді температурної хвилі, в атомарному бозе-конденсаті другий звук є коливанням густини конденсату.

ФЕНОМЕНИ ПРИРОДИ: ФІЗИЧНІ МОДЕЛІ ТА ЇХ СТУПІНЬ КОРЕЛЯЦІЇ З РЕАЛЬНІСТЮ

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Аналіз специфіки традиційних форм навчального процесу і проведення предметних олімпіад, як основної форми роботи з найкращими учнями, дає змогу зробити висновок, що виконання абстрактних, часто відірваних від реалій життя задач, вправ і завдань за відведений на це час не збігається зі специфікою наукової роботи, в якій найважливіше – вдало обрати проблему та розв'язати її, часто завдяки тривалій, систематичній праці.

Саме такого підходу вимагають проблемні задачі (задачі Капіци), які пропонуються на турнірах юних фізиків (ТЮФ). Завдання турніру – це, як правило, нестандартні задачі. Більшість із них, по суті, є науковими або навчальними проблемами і вимагають проведення справжніх досліджень: починаючи від припущень і моделі опису і закінчуючи аналізом отриманих результатів.

Тому метою цього дослідження є пошук шляхів розв'язання та їх обґрунтування на деякі проблемні завдання, запропоновані на XIX Всеукраїнському ТЮФ.

Предметом дослідження стали 4 завдання:

1. «Рибальський ліхтар». Виготовте ліхтар зі звичайної свічки і пластикової пляшки. За яких співвідношень розмірів частин ліхтаря він працюватиме надійно?

2. «Кам'яні оракули». Дослідники дольменів висловили гіпотезу, що дольмени попереджали про наближення землетрусів. Проаналізуйте цю гіпотезу.

3. «Вікінги». Згідно з легендою, вікінги вміли орієнтуватися в океані навіть у похмуру погоду, використовуючи кристали турмаліну. Як можна здійснити навігацію в похмуру погоду за допомогою турмаліну? Яка точність використовуваного методу?

4. «Задача Аргонавтів». Чому окремі краплі можуть рухатися поверхнею води, як кульки? Дослідіть експериментально цей ефект, опишіть його теоретично.

Виконання завдань здійснювалося за схемою:

• пошук першоджерел умови задачі (якщо вона має історичний

аспект);
- проведення експерименту (якщо це можливо);
- пропонування гіпотез та ідей;
- якісний та кількісний опис;
- створення фізичної моделі;
- аналіз теоретично отриманих результатів і порівняння з результатами експерименту;
- висновок.

На основі проведеної роботи отримано такі результати:

1. «Рибальський ліхтар». Розглянуто процеси теплообміну, визначено умови стабільної роботи ліхтаря, обґрунтовано параметри і співвідношення розмірів пляшки та свічки.

2. «Кам'яні оракули». Змодельовано процес: дольмен розглянуто як резонатор Гельмгольца. На основі одержаних результатів отримано підтвердження реалістичності гіпотези, запропонованої в умові задачі.

3. «Вікінги». Уточнено умову легенди-першоджерела, оцінено реальність орієнтування вікінгів завдяки «чудо-каменю», запропоновано спосіб навігації за допомогою кристалу турмаліну й оцінено точність методу.

4. «Задача Аргонавтів». Ефект перевірено експериментально, запропоновано ідею його теоретичного обґрунтування на основі явища поверхневого натягу, теоретична оцінка якісно узгоджується з результатами експерименту.

Висновки: проаналізовано фізичні явища і процеси в поставлених завданнях; запропоновано можливі способи розв'язання чотирьох проблемних завдань, створено описові моделі, отримано якісні та кількісні результати, які підтверджено експериментально.

ДОСЛІДЖЕННЯ ПРИСКОРЕННЯ ФЕРОМАГНІТНИХ ТІЛ ПІД ДІЄЮ ЕЛЕКТРОМАГНІТНОГО ПОЛЯ

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В работе рассмотрены теоретические основы накопления и высвобождения электрической энергии в электромагнитной пушке (ЭМП). Разработаны и исследованы различные способы управления движением ферромагнетика в магнитном поле.

Предложен и проверен оценочный теоретический расчет параметров катушки для конкретной установки, способной сообщать максимальную скорость снарядам из ферромагнетика.

Изучены принципы работы ЭМП, где накопителем являются конденсаторные батареи.

Разработан проект малогабаритной, низковольтной, безопасной ЭМП.

Удалось создать оригинальную низковольтную безопасную ЭМП, способную с помощью тяжелых ферромагнетиков ускорять маленькие диамагнитные снаряды до скорости в два раза большей, чем скорость самих ферромагнетиков.

Созданное устройство может быть использовано не только в тире для тренировки, а и на уроках физики при выполнении лабораторных работ физического практикума при изучении темы электромагнетизма или движения тел в поле притяжения земли.

Получены выводы, что реально осуществимы два основных пути увеличения конечной скорости разгона ферромагнетика:

• большая емкость конденсаторов, низкое напряжение и большое количество витков проволоки в катушке;

• высокое напряжение, средняя емкость конденсаторов и мало витков толстого провода в катушке.

В работе изучены и апробированы оба представленных способа, получены результаты, близкие к теоретическим и экспериментально исследованые.

ЛЕГУВАННЯ НАПІВПРОВІДНИКІВ МЕТОДОМ ТЕРМІЧНОЇ ДИФУЗІЇ

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Термодифузійний ефект був відкритий Л. Дюфуром ще у 1873 році. Прямий термодифузійний ефект (для газів) полягає в тому, що за наявності постійної різниці температур по обидва боки перегородки, що розділяє один і той самий газ, виникає, зростає і стає постійною різниця тиску, навіть якщо спочатку її не було. Отже, різниця (градієнт) температур приводить до різниці (градієнту) концентрацій. Це явище і є термодифузією.

Дифузія легуючих домішок у напівпровідникові кристали ввійшла у промислове виробництво з 1960-х років і до сьогодні є основним технологічним методом створення електрично-гетерогенних структур при виготовленні різних типів напівпровідникових приладів та інтегральних мікросхем (ІМС). Для здійснення дифузії напівпровідникову пластину розташовують у нагрітій до високої температури кварцовій трубі дифузійної печі. Через трубу пропускають пари легуючої домішки, що адсорбуються на поверхні пластини і дифундують у кристалічні ґратки напівпровідника.

У практиці технологічних розрахунків дифузійних структур значне поширення одержали задачі з визначення профілів розподілу домішок за заданими режимами дифузії і зворотні задачі – визначення тривалості й температури дифузії за відомим типом домішки, її концентрації і глибині залягання p-n-переходу. У цій роботі ми зробили першу спробу опанувати методику розрахунку параметрів термічної дифузії – побудували розрахунковий профіль розподілу фосфору в кремнії. Визначено також, що глибина залягання p-n-переходу в цьому випадку становить ~ 1,89–5,1 мкм.

ВИКОРИСТАННЯ БЛОК-СХЕМ ПРИ РОЗВ'ЯЗУВАННІ ЗАДАЧ ІЗ ФІЗИКИ. ЕЛЕКТРОННИЙ ПОСІБНИК З ФІЗИКИ

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Використання інформаційних технологій – це вимога часу. Зв'язок фізики з інформатикою та іншими галузями науки є важливим. Фізика є одним із предметів, який сприяє формуванню інтелектуально розвиненої особистості, а розв'язування нестандартних задач сприяє розвитку розумових і творчих здібностей учнів.

Мета роботи: розроблення алгоритму, який оптимізовує розв'язування таких задач, дає змогу отримати правильний результат у найбільш раціональний спосіб.

Розглянуто п'ять задач із різних розділів фізики. Вибрані типові задачі, в яких учні припускаються найбільше помилок. До кожної з них дається теоретичне обґрунтування фізичних процесів і закономірностей, пропонуються два способи розв'язування: словесно-формульний алгоритм і використання блок-схеми. Оскільки останній спосіб є дуже наочним і доступним, йому приділяється особлива увага. Пункт «презентація» дає змогу ознайомитися з типовими помилками, яких припускаються учні при розв'язуванні задач. Пункт «діаграма» дає змогу проаналізувати покрокове виконання блок-схеми для різних початкових даних.

Програми мовою Паскаль дають змогу здійснювати самоконтроль при перевірянні результатів обчислень. Програми мовою Delphi дають змогу користувачеві працювати з комп'ютером в інтерактивному режимі.

Для кращої наочності і привабливості до більшості із запропонованих у роботі задач створені відповідні флеш-анімації.

ЕКСКУРС У ХВИЛЬОВУ ОПТИКУ

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У житті ми часто стикаємося з певними явищами, які не можемо пояснити. Одне з таких явищ – отримання просторових зображень за допомогою голограм. Оскільки дослідження голограм неможливе без знання хвильової оптики, то ми вирішили включити у свою роботу ще й теоретичні відомості з цього розділу фізики.

Мета роботи: створення програми, яка б дала змогу користувачеві отримати коротку, наочну і зрозумілу інформацію про хвильову оптику, детальну інформацію про голограми, їх моделювання та виготовлення; розроблення програми, яка дасть змогу користувачу змоделювати голограму і дослідити її залежність від різних параметрів, навіть не маючи глибоких знань із цього питання.

Програма зберігає дані, введені користувачем, і виводить перелік об’єктів, доданих користувачем у відповідний список. Після натискання на кнопку «Розрахувати» програма починає моделювати голограму. Для того щоб розрахувати голограму, програма вважає кожен із доданих користувачем об’єктів джерелом світла, фокусатор у точку – точковим джерелом світла, фокусатор у лінію – прямою, що світиться, тощо. Далі за наведеними у розділі «Моделювання голограм» формулами розраховується інтерференційна картина на екрані, шляхом розрахунку інтенсивності світла в кожній точці екрану, враховуючи при цьому довжину хвилі для монохроматичного світла. Відтак отримана інтенсивність перетворюється у відтінок відповідного кольору так, щоб мінімальній інтенсивності відповідав чорний колір, а максимальній – найяскравіший відтінок цього кольору. У такому вигляді картина виводиться на екран, і користувач бачить отриману голограму.

ТЕОРІЯ ГРУП І ЕЛЕМЕНТАРНІ ЧАСТИНКИ

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Актуальність дослідження. Останнім часом актуальною темою є завершення формування Стандартної моделі елементарних частинок. Від цього залежить подальший розвиток теоретичної і, перш за все, практичної науки. Дотепер усі прогнози Стандартної моделі підтверджувалися експериментами, іноді з фантастичною точністю в мільйонні частки відсотка. Тільки останніми роками почали з'являтися результати, в яких прогнози Стандартної моделі дещо розбіжні з експериментами. З іншого боку, очевидно, що Стандартна модель не може бути останнім словом у фізиці елементарних частинок, бо вона містить дуже багато зовнішніх параметрів, а також не включає гравітацію. Тому пошук відхилень від Стандартної моделі — один із найактивніших напрямів дослідження останніми роками.

Об'єкт дослідження: Стандартна модель у фізиці елементарних частинок.

Мета роботи: дослідити Стандартну модель у фізиці елементарних частинок і показати застосування в ній теорії груп.

Відповідно до мети визначено такі завдання дослідження:
- дослідити групу Лі;
- дослідити спеціальну унітарну групу SU(n);
- дослідити Стандартну модель.

У роботі досліджено:
- групу Лі;
- спеціальну унітарну групу SU(n);
- Стандартну модель.

Застосування пропонованої теми. Наукове значення Стандартної моделі полягає не тільки у її здатності описувати фундаментальні властивості елементарних компонентів Усесвіту, а є наслідком успіхів її застосування в астрофізиці й космології моделями, заснованими на загальній теорії відносності, до опису властивостей Всесвіту в космологічних масштабах.

Висновки. Працюючи над цією темою, ми намагалися дослідити Стандартну модель у фізиці елементарних частинок і показати застосування в ній теорії груп. Ми вважаємо, що Стандартна модель є значним успіхом наукової думки, проте є неповною, і треба очікувати подальшого її розвитку.

Секція «Астрономія та астрофізика»

СОНЯЧНА АКТИВНІСТЬ ТА ЇЇ ВПЛИВ НА ФУНКЦІОНАЛЬНІ СИСТЕМИ ОРГАНІЗМУ

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Метою роботи є дослідження й аналіз залежності кількості випадків захворювань серцево-судинної системи від сонячної активності. Адже під час високої активності Сонця загострюються хвороби. Тому вивчення активності Сонця і запобігання її шкідливому впливу є дуже актуальним питанням.

Сонце – гаряча плазмова куля, в ядрі якої відбуваються термоядерні реакції, що є джерелом енергії.

Сонячна активність визначається сукупністю фізичних змін, які відбуваються на Сонці. Її зовнішні прояви – сонячні плями, протуберанці, факели тощо. Число Вольфа – основний індекс сонячної активності, що відображає кількість плям і груп плям на Сонці. Сонячна активність у числах Вольфа має циклічний характер із середньою тривалістю циклу в 11,2 року.

Активність Сонця найбільше впливає на серцево-судинну та нервову системи. Магнітна буря супроводжується зменшенням скоротливої сили серця. Висока сонячна активність має гальмівну дію на ракові клітини.

Двадцять четвертий цикл сонячної активності характеризується винятково повільним початком утворення і збільшення сонячних плям.

Досліджуючи залежність кількості випадків серцево-судинних захворювань від активності Сонця, за основу для порівняння було використано статистику пацієнтів Тячівської РЛ № 1 – хворих на гіпертонічну хворобу, ішемічну хворобу серця і гострий інфаркт міокарда.

Загострення гіпертонічної та ішемічної хвороб прямо пропорційно залежить від активності Сонця, а інфаркту міокарда – обернено пропорційно. Також наприкінці кожного року спостерігається зниження кількості випадків хвороб серцево-судинної системи.

ПРОЕКТ: ЧАС, ЙОГО ВИМІРЮВАННЯ ТА ВИКОРИСТАННЯ

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У роботі йдеться про те, що облік часу – одне з основних і найдавніших завдань астрономії. Наголошено на важливості цієї одиниці виміру в нашому чотиривимірному просторі.

Мета роботи: дізнатися більше про час як вимір, як важливу одиницю в нашому чотиривимірному світі, відкрити для себе щось нове у повсякденному житі; звернути увагу однолітків на цю важливу форму вимірювання, зацікавити їх, добиватися, щоб вони раціонально використовували час.

У роботі йдеться про різні види годинників: біологічний, сонячний, пісочний, водяний, механічний, маятниковий, астрономічний, хронометр, електронний та атомний. Біологічний ґрунтується на циклічних ритмах живих організмів. Основою сонячного є видимий рух Сонця небосхилом і його висота над горизонтом. Основним циклом пісочного і водяного годинників є періоди переміщення з однієї посудини до іншої відповідно піску та води. Робота механічного годинника ґрунтується на періоді, за який опускається гиря, тим самим повертаючи вал, на який була намотана. Принцип дії маятникового годинника полягає в тому, що вантаж, підвішений за допомогою шнура, намотаного на вал, створює силу, що рухає всю систему коліс, а маятник забезпечує рівномірність їх ходу. Основним в астрономічному годиннику є секундний маятник, який здійснює одне коливання в секунду, і механізм, що веде відлік коливання маятника. Рушійною силою в хронометрі є сильна спіральна пружина, а регулятором руху стрілок – балансир, що коливається то в один, то в інший бік під дією слабшої спіральної пружини. В електронному годиннику для відліку часу використовуються періодичні коливання електронного генератора (зокрема у Вінницькому національному технічному університеті знаходиться оптико-електронний годинник, що працює на квантово-розмірних структурах – сучасних над'яскравих світлодіодах). В атомному годиннику як періодичний процес використовуються власні коливання атомів або молекул. Також у роботі йдеться про пасажний інструмент як прилад для знаходження поправки для годинника.

Досліджено різні види часу, зокрема справжній сонячний і середній сонячний, надаються формули для їхнього обрахунку. Пояснюється, чим вирізняються місцевий і поясний час, згадується лінія зміни дат. Також висвітлюються відмінності між літнім і декретним часом, подається історія їх запровадження.

Основні цикли, що використовуються при складанні календарів: доба, тропічний рік і синодичний місяць. Основні види календарів: сонячний, місячний і сонячно-місячний.

Плин часу незмінний і постійний, сучасна наука не в змозі його підкорити, а лише виміряти. Наголошено на раціональному використанні часу в повсякденному житті, на необхідності берегти і цінувати свій час і час співрозмовника.

ФОТОГРАФІЧНІ СПОСТЕРЕЖЕННЯ МЕТЕОРНИХ ПОТОКІВ

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Робота присвячена вивченню методів спостереження метеорних явищ, фотографуванню метеорів і створенню устаткування для фотографічних спостережень.

Метеори належать до короткочасних явищ природи. Крім того, заздалегідь невідомо, в якій ділянці піднебіння і в який момент пролетить метеор. У цьому полягає складність спостережень метеорів.

Найдоступнішим наразі є фотографічний метод спостережень метеорів. Він дає змогу визначити всі візуальні параметри метеора. Перевага його перед візуальним методом полягає в тому, що в нім відсутній людський чинник і результати є достовірнішими.

Мета роботи: освоїти фотографування метеорів і здійснити зйомку метеорних потоків з паралельними візуальними спостереженнями за програмою «Загальний огляд радіантів».

Було здійснено три поїздки для фотоспостережень Оріонідів, Леонідів (2009) і Персеїдів (2010). Для фотографування використовувалися дзеркальні фотоапарати «Зеніт», які кріпилися на фотоштативі, майданчиках телескопів «Міцар» і метеорному патрулі. Кількість фотографій з метеорами – 15, найбільш яскравих (яскравіше третьої зоряної величини) – 6.

РЕЛЬЄФНІ ОСОБЛИВОСТІ ПОВЕРХНІ ТА ФОРМА АСТЕРОЇДІВ

Каценко Тетяна Сергіївна

учениця 10 класу ліцею № 15 м. Чернігова

Дослідження фізичних властивостей астероїдів має фундаментальне значення для розв'язання проблеми походження й еволюції Сонячної системи. У зв'язку з освоєнням космосу і плануванням польотів до малих планет різко зросла потреба в інформації про фізичні характеристики астероїдів.

На сьогодні у суспільстві багато уваги приділяється проблемі можливого зіткнення астероїдів різного розміру із Землею, необхідності побудови глобальної системи спостереження й оповіщення про небезпечні астероїди, методи протидії зіткненням.

У цій роботі було досліджено, як впливають на вигляд кривої блиску астероїда різні геологічні утворення, а саме: гірські утворення, кратери, фотометрична неоднорідність поверхні астероїда, а також як змінюється крива блиску від кута аспекту. Дослідження проводилися на зібраній власноруч установці. За базову модель астероїда взяли тривісний еліпсоїд, на якому моделювались ті чи інші геологічні утворення та фотометричні неоднорідності. Для різних моделей астероїдів були отримані їх криві блиску при різних кутах аспекту.

Після аналізу отриманих даних було визначено з деякою імовірністю форми таких астероїдів: 92Undina, 599Luisa, 551Ortrud, 216Kleopatra, 1602Indiana, 559Nanon, 8Flora, 6446Chruanta.

ФОТОМЕТРІЯ АСТЕРОЇДА 16 PSYCHE В ОПОЗИЦІЮ 2010 РОКУ

Котелевець Микола Анатолійович

учень 9 класу комунального закладу "Іванівський навчально-виховний комплекс" Чугуївської районної ради Харківської області

У роботі зроблений огляд літератури з досліджень астероїда основного поясу 16 Psyche, який за таксономічною класифікацією належить до нечисленної групи М-астероїдів (металевих). Наведені результати нових фотометричних спостережень астероїда у стандартних спектральних смугах BVR і I, які були виконані у жовтні-грудні 2010 року на 70-сантиметровому рефлекторі Чугуївської спостережної станції Інституту астрономії ХНУ імені В. Н. Каразіна. Фотометрія була виконана за допомогою панорамного приймача випромінювання ПЗЗ-камери ML 47-10. За результатами фотометрії одержані криві блиску в кожній із спектральних смуг, які мають амплітуду варіацій блиску 0.m14. Було показано, що відсутні варіації показника кольору V-R по поверхні астероїда при південному аспекті спостереження астероїда. Той факт, що, за літературними даними, при північному аспекті мають місце варіації V-R, а, за нашими даними, при південному аспекті їх немає, визначає місце розташування на поверхні Psyche фотометричного утворення, а саме – у північній півкулі цього астероїда.

КАЛЕНДАРНІ ЗАКОНОМІРНОСТІ

Нежура Владислав Юрійович

учень 9 класу Запорізького технічного ліцею

Робота присвячена дослідженню календарних закономірностей. Коротко розглянуто різні види календарів, що існують (або існували). Особливу увагу приділено дослідженню григоріанського календаря, яким ми нині користуємось.

Показано, що григоріанський календар є далеким від досконалості. Його мінуси – це місяці і квартали різної тривалості, розбіжність дат і днів тижня в різних місяцях. Цей календар неточний, за досить тривалі проміжки часу накопичується помилка. Неточність можна пояснити низьким рівнем розвитку математики й астрономії на час створення календаря. Недоліки григоріанського календаря є причиною різних незручностей.

Нині існують більш досконалі проекти календарів, які заслуговують на увагу. Це всесвітній постійний календар і стабільний календар. Вони точніші та зручніші. Однак спроби їх запровадити зіткнулися з релігійними і національними традиціями.

У процесі виконання роботи було знайдено багато закономірностей григоріанського календаря.

Встановлено закономірність чергування річних календарів. Розв'язано задачу конкретизації періоду життя, описаного у вірші Й. Бродського.

Показано, як можна розв'язати проблему календаря за допомогою ланцюгових дробів.

Знайдено і перевірено деякі алгоритми для знаходження дня тижня по даті.

Розв'язано ряд конкретних задач, зокрема задачу про т. зв. «чорну п'ятницю».

Вважаємо, що наша робота може використовуватися на позакласних заняттях як з астрономії, так і з математики.

ЕЛЕКТРОННА ЕНЦИКЛОПЕДІЯ "ГАЛАКТИКИ"

Свіженко Андрій Олегович

учень 10 класу комунального закладу освіти "Дніпропетровського ліцею інформаційних технологій при Дніпропетровському національному університеті імені Олеся Гончара"

Галактики – гігантські (до 10^{13} зірок) зоряні системи, розташовані поза межами нашої Галактики. Також їх іноді називають позагалактичними туманностями, бо при візуальному спостереженні у телескоп вони виглядають туманними плямами, як і звичайні газові туманності.

Дані про галактики наводяться у спеціальних астрономічних каталогах. З них найвідомішими є перший каталог туманностей і зоряних скупчень, складений наприкінці XVIII століття французьким астрономом Ш. Месьє (у цьому каталозі туманність Андромеди, наприклад, записана під номером 31 і позначається як М31), і «Новий загальний каталог» (1888) ірландського астронома Дж.-Л.-Е.-Дрейера (скорочено NGC, у ньому, наприклад, туманність Андромеди позначається NGC 224).

Світ зоряних систем – галактик – почав інтенсивно вивчатися з 1920 р., коли шведському астроному К. Лундмарку вдалося розкласти на окремі зірки периферійну частину спіральної галактики М33 (або NGC 598) у сузір'ї Трикутника. Незабаром американський астроном Е. Хаббл, працюючи на найбільшому на той час телескопі із дзеркалом діаметром 2,5 м, визначив зоряну природу спіральних рукавів туманності Андромеди і декількох більш слабких галактик неправильної форми. Це поклало початок розвитку нової гілки астрономічної науки – позагалактичної астрономії.

Вивчення галактик потребує максимально потужних інструментів, наприклад, оптичних телескопів із дзеркалами діаметром більше метра, а також найновіших засобів і методів дослідження далеких слабких об'єктів. Винятково швидкому розвитку позагалактичної астрономії сприяло запровадження радіоастрономічних методів дослідження космічних об'єктів.

Позагалактична астрономія досліджує розміри зоряних систем, їх маси, будову, властивості оптичного, інфрачервоного, рентгенівського і радіовипромінювання. Вивчення просторового розподілення галактик виявляє великомасштабну структуру Всесвіту. У дослідженні

просторового розподілення галактик і шляхів їх еволюції позагалактична астрономія зливається з космологією – наукою про Всесвіт загалом.

Висновки.

У процесі роботи було опрацьовано чимало літератури про фізику, астрономію і космологію. Поєднавши вивчений матеріал, ми створили комп'ютерну енциклопедію, у яку вмістили основну інформацію з досліджених тем і моделювальну програму, присвячену гравітаційним полям.

Пропоновану роботу можуть використовувати викладачі ліцеїв, гімназій і шкіл для викладання деяких тем з астрономії та фізики, а також учні для підготовки рефератів і доповідей, вивчення астрономії і фізики. Також ця робота може стати у пригоді будь-якій людині, що цікавиться астрономією або фізикою.

Секція «Аерофізика та космічні дослідження»

ВИМІРЮВАННЯ ЗАГАЛЬНОГО ВМІСТУ ОЗОНУ НА СТАНЦІЇ КИЇВ-ГОЛОСІЇВ

Гладіков Денис Костянтинович

учень 9 класу ліцею № 100 "Поділ" м. Києва

Мета роботи: дослідити загальний вміст і динаміку озону на станції Київ-Голосіїв за допомогою спектрофотометра Добсона.

Завдання роботи: вивчити будову спектрофотометра Добсона і методики проведення вимірювань; провести вимірювання загального вмісту озону на станції Київ-Голосіїв; зібрати й опрацювати результати вимірювань; зробити висновки.

Робота є актуальною, оскільки до сьогодні на території України вимірювання загального вмісту озону за допомогою спектрофотометра Добсона не проводилися, а цей прилад має більшу точність, ніж наявні в Україні озонометри М-124. Озон відіграє важливу роль у збереженні біосфери нашої планети, тому контролювати його кількість дуже важливо. Оскільки основні озоноруйнівні речовини можуть міститися в атмосфері роками, то можливі наслідки діяльності людини треба розраховувати наперед.

ЗАСТОСУВАННЯ ОРБІТАЛЬНИХ ТРОСОВИХ СИСТЕМ

Кохан Максим Сергійович

учень 10 класу ліцею № 15 м. Чернігова

Основною відмінністю орбітальних тросових систем від традиційних космічних апаратів є їхня велика довжина, яка може сягати десятків і сотень кілометрів, а в деяких випадках навіть тисяч і десятків тисяч кілометрів, зі збереженням при цьому механічного, енергетичного та інших зв'язків між кінцевими тілами. Саме здатність тросів створювати протяжні космічні системи й обумовлює ряд чудових властивостей цих систем. По-перше, можливість більш сильної взаємодії із зовнішніми полями планети, по-друге, можливість змінювати швидкість космічних апаратів без використання палива, по-третє, можливість використання магнітного поля Землі та її іоносфери для вироблення електроенергії чи зміни орбіти космічних апаратів.

У цій роботі розглядається принцип безпаливного збільшення швидкості космічних апаратів, застосовуючи при цьому енергію обертової тросової системи.

Розрахунки свідчать про можливість використання динамічних тросових систем для виконання певних операцій у космосі, де тросові системи змогли б знайти ефективне застосування.

КОСМІЧНІ НЕБЕЗПЕКИ ДЛЯ ЗЕМНОЇ ЦИВІЛІЗАЦІЇ

Лук'яненко Станіслав Миколайович

учень 9 класу Харківського приватного навчально-виховного комплексу "Старт-школа" Харківської області

У роботі розглянуті реальні і потенціальні космічні небезпеки та їхній імовірний вплив на Землю. Виконаний аналіз проблем, пов'язаних з можливістю зіткнення з Землею астероїдів і комет. Проведені розрахунки розміру кратера при падінні на Землю астероїдів радіусом 25, 500 і 5000 м. Зроблений аналіз наслідків для Землі кінцевих стадій еволюції Сонця і можливого вибуху надової поряд із Сонячною системою. Наведений список ділянок Галактики, у яких можливий вибух надових II типу. Розглянута проблема космічного сміття, небезпек, пов'язаних із сонячною активністю. Виконаний аналіз захисної функції атмосфери Землі від короткохвильового випромінювання Сонця та інших космічних об'єктів.

Особлива увага приділена озоновій проблемі. Зроблені оцінювання зміни величини пропускання УФ-випромінювання земною атмосферою за рахунок зменшення шару озону.

ПІДВИЩЕННЯ ЕФЕКТИВНОСТІ ДОСЛІДЖЕННЯ ПЛАНЕТИ МАРС ШЛЯХОМ КОМПЛЕКСНОГО ЗАСТОСУВАННЯ МОБІЛЬНОГО КОМПОНЕНТУ БЕЗПРОВІДНИХ СЕНСОРНИХ МЕРЕЖ

Орленко Сергій Петрович

учень 10 класу Пирятинського ліцею Полтавської області

З настанням ери космічних польотів стало можливим перевести астрономічні дослідження найближчих до Землі космічних об'єктів від пасивного спостереження в площину активного дослідження й отримання конкретних результатів безпосередньо з їхньої поверхні. Одним із перспективних напрямів досліження можна вважати впровадження технології розподілених безпровідних сенсорних мереж і включення до їх складу мобільного компоненту, як фактора, що має підвищити ефективність застосування останніх.

Розподілені безпровідні сенсорні мережі мають ряд переваг у порівнянні з традиційними системами збирання даних. Однією з них є можливість застосування такої технології при збирання даних у багатьох точках визначеної частини поверхні, що допоможе дослідити зміни параметрів досліджуваних об'єктів на заданій території, властивості атмосфери, тощо.

Безпровідна сенсорна мережа – це набір інтелектуальних сенсорів, розміщених на певній території та об'єднаних у систему збирання даних протоколом обміну і відповідними власними й мережними технічними характеристиками. Ефективність функціонування такої дослідницької мережі можна підвищити за рахунок введення до її складу мобільного компоненту – вузла, розміщеного на рухомій платформі, що керується автономною мікропроцесорною системою. Взаємодіючи зі стаціонарними вузлами, мобільний компонент може вільно переміщуватися в межах їх "видимості", виконувати завдання збирання даних у проблемних зонах, які є недоступними для закріплених вузлів. Ефективність мережі може бути ще вищою, якщо в її складі буде кілька мобільних компонентів. Взаємодіючи між собою, вони можуть узгоджено змінювати своє місцеположення і вести системні дослідження подібно до колонії мурашок.

Варто наголосити і на дешевизні таких систем і зручності їхнього розгортання, що може здійснюватися без участі людини. Це особливо актуально для тих ситуацій, коли присутність людини є або принципово неможливою, або небезпечною.До уваги пропонується діючий прототип мобільного компоненту розподіленої сенсорної мережі.

РОЗРАХУНОК ТРАЄКТОРІЙ ПОЛЬОТУ КОСМІЧНОГО АПАРАТУ З ІОННИМ ДВИГУНОМ З НАВКОЛОЗЕМНОЇ ОРБІТИ ДО МІСЯЦЯ

Пицко Наталія Ярославівна

учениця 10 класу Калуської гімназії Калуської міської ради Івано-Франківської області

Метою пропонованої роботи є розрахунок траєкторії руху космічного апарата (КА) з навколоземної орбіти до Місяця відносно центра мас системи Земля–Місяць. Оскільки під час руху КА на нього діятимуть, крім сил гравітації з боку Сонця, Місяця і Землі, ще й сили інерції, то для розрахунку траєкторії потрібно застосувати чисельні методи розв'язку диференційних рівнянь, яких існує досить багато.

Серед них вибрано найпростіший метод Тейлора, але в системі координат, що обертається.

Виведено послідовність формул, що дають змогу знайти швидкість і положення КА в будь-який момент часу.

Складено програму для розрахунку траєкторій і виведення їх на монітор.

Зроблено також аналіз отриманих результатів:

• наш метод у такому вигляді, як він представлений у роботі, дає змогу розраховувати наближені траєкторії руху небесних тіл;

• найперспективнішим є рух КА з виведенням на геостаціонарну орбіту з розділенням його на дві частини, одна з яких рухається по цій орбіті і використовується як супутник зв'язку, а інша за допомогою іонного двигуна дістається Місяця, стає його штучним супутником або стає штучним супутником Землі, якщо Місяць не зможе втримати її.

Наш метод можна зробити більш точним, зменшивши крок Δt, а також урахувавши неоднорідність гравітаційних полів.

СТАРТ РАКЕТИ З ПОВІТРЯНОЇ ПЛАТФОРМИ

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Мета роботи: розроблення проекту старту космічних ракет з повітряної стратосферної платформи; розгляд можливості реалізації цього проекту, доведення його технічних, екологічних та економічних переваг.

Густонаселені європейські країни не мають можливості будувати велетенські наземні космодроми, принаймні на своїй території. Серед нових варіантів стартів космічних ракет найкращим може стати створення стратосферної стартової платформи. Збудувавши таку платформу, ми отримуємо «космодром», який не тільки високо розташований, а й здатний маневрувати, обираючи найбільш вигідну точку старту, робити попередній розгін. Такий старт має екологічні переваги – потребує менше палива, яке, до того ж, згоратиме на висоті, запобігаючи тим самим осіданню продуктів згоряння на поверхні Землі. Відпадає потреба у великих площах, яких потребує наземний космодром.

У роботі розглянуто будову атмосфери, прорахована залежність сили тяжіння від висоти над поверхнею Землі. Обрана висота старту становить 20–30 км. Показано, що простий підйом на цю висоту зменшить стартову вагу на декілька тонн для ракети стартовою вагою в декілька сотень тонн. Це сприяє економії при будуванні ракети або дає змогу збільшувати її корисний вантаж.

Розраховані об'єми балонів для запропонованої платформи. Розглянута будова і методи використання стартової платформи.

Розроблення проекту потребує подальших теоретичних розрахунків і практичних досліджень.

МЕТЕОРИТИ. ІЛЛІНЕЦЬКИЙ МЕТЕОРИТ

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Мета дослідження: вивчити основні характеристики метеоритів, дослідити Іллінецький метеорит і його характеристики як одного з представників малих тіл Сонячної системи, що потрапили на Землю.

Актуальність. Дослідження метеоритів є важливим напрямом наукової діяльності в галузі палеонтології, космології та геологічної історії. На порядку денному стоїть вивчення геологічних, біологічних наслідків падіння метеоритів в океани й моря. Безсумнівно, що саме на цьому шляху знайдуться відповіді на запитання про механізми і причину швидких змін у складі тваринного й рослинного світу Землі і, можливо, про походження життя взагалі.

Астроблеми — великі кратероподібні кільцеві утворення на поверхні Землі, кратери остаточно не визначеного походження. За складом метеорити поділяються на залізні, залізо-кам'яні і кам'яні.

Нині на нашій планеті існує близько 10 тисяч земних "шрамів", але з упевненістю астроблемами називають лише 110–150 геологічних структур. Із них сім знаходяться в Україні: Бовтиська, Іллінецька, Оболонська, Ротмістрівська, Тернівська, Біллівська, Зеленогайська.

При огляді і частковому дослідженні території Іллінецького кратера було зроблено світлини місцевості, виміряно потужність радіації (0,3 мкЗв/год), густину цього об'єкта (2,454 г/см^3), з відносною похибкою 1,474%; виміряно товщину кірки плавлення (0,8–1 мм), нашарування ґрунту над об'єктом дослідження.

У навчально-науковому центрі фізико-хімічних досліджень при ЧНУ було проаналізовано хімічний склад зразка цоколя метеориту за рентгеноспектральним і рентгеноструктурним аналізами. Було зроблено порівняльну характеристику хімічного складу зазначеного зразка зі зразками геологічних структур, характерних для цієї місцевості зі схожим хімічним складом. Зразки цоколя метеориту розглядалися під електронним мікроскопом МБС-9. При цьому в зразку були виявлені частинки кварцу, оксидів Феруму, вкраплення заліза і помічені хондрити.

Результати досліджень доводять, що цей об'єкт є метеоритною структурою Українського щита і проявляє ознаки ударного метаморфізму.

ВИЗНАЧЕННЯ ВМІСТУ ШКІДЛИВИХ КОМПОНЕНТІВ (ЙОНІВ СТРОНЦІЮ ТА ЙОНІВ РТУТІ) У ТОВАРАХ ПЕРШОЇ НЕОБХІДНОСТІ ТА ПРОДУКТАХ ХАРЧУВАННЯ МЕТОДОМ СПЕКТРАЛЬНОГО АНАЛІЗУ

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Спектральний аналіз був відкритий Г. Кірхгофом та Р. Бунзеном в 1859 році, які довели, що розпечені пари кожного елемента давали промені строго певного кольору і призма відхиляла ці промені на строго певне місце, і тому ні один колір не міг замаскувати іншого.

Спектральний аналіз вже в минулому столітті допоміг досліджувати склад Сонця та інших зірок, а також відкрити деякі елементи, зокрема гелій. За допомогою спектрального аналізу стало можливим відрізняти не тільки різні хімічні елементи, але й ізотопи одного й того ж елементу, які зазвичай дають неоднакові спектри. Метод застосовується для аналізу ізотопного складу речовин.

Спектроскопія відкриває різносторонні можливості для досліджень у біології, біохімії, астрономії, інших галузях науки і техніки.

Йони ртуті та стронцію небезпечні для людини. Ртуть легко випаровується, а її пари, потрапляючи в легені, повністю затримуються там і викликають згодом отруєння організму, хоча й не таке швидке, як солі ртуті.

Потрапляючи в ґрунт, стронцій разом з розчинними сполуками кальцію надходить у рослини. Більше за інших накопичують стронцій 90 бобові рослини, корені і бульбоплоди, менше – злаки, у тому числі зернові і льон.

Дослідження товарів щоденного вжитку показує, що у деяких з вибраних зразків виявлено йони стронцію та ртуті.

ТЕПЛОПРОВІДНІСТЬ

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Навколо нас відбуваються різні види теплових процесів. Перебіг теплових процесів відбувається, як правило, таким чином, що це позначається на зміні внутрішньої енергії тіл. Якщо тіло нагрівається, то середня кінетична енергія його молекул зростає, оскільки підвищується температура тіла і швидкість молекул збільшується. Отже зростає внутрішня енергія тіла. І, навпаки, якщо тіло охолоджується, внутрішня енергія зменшується. Але ми знаємо, що змінити температуру тіла можна виконанням механічної роботи і внаслідок передачі теплоти. Передавання енергії від одних тіл до інших внаслідок теплообміну є одним з найпоширеніших процесів у навколишньому світі.

Одним із видів теплообміну (теплопередачі) є теплопровідність. Теплопровідність – це здатність тіл проводити тепло. Одні тіла добре проводять тепло, а інші погано.

Вчені давно пояснили теплопровідність тіл на основі уявлень про атомно-молекулярну будову речовини.

Дана робота складається із вступу, трьох розділів, висновків, додатків.

У роботі пояснено механізм теплопровідності речовин у різних агрегатних станах на основі атомно-молекулярних уявлень про будову речовини із дослідним обґрунтуванням. Описано дослідження теплопровідності ґрунтів даної місцевості.

Крім того, висвітлено питання про коефіцієнт речовини, описано метод експериментального визначення коефіцієнта теплопровідності ґрунту.

Описано і наведено факти про добрі і погані провідники тепла та використання їх людиною; про роль теплопровідності в життєдіяльності людини.

Описана інформація, яка отримана в процесі дослідження теплопровідності може бути використана у різних видах діяльності.

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SPECTRAL CHARACTERIZATION AND SOME PROPERTIES OF PARTIALLY ALIPHATIC POLYIMIDES

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Among the high-performance polymers, polyimides present a great importance due to their superior thermal and mechanical properties, which make them useful for advanced technologies [1,2]. In this work, novel polyimides were prepared using aliphatic monomers in order to reduce charge transfer interactions and implicitly to improve solubility, optical and dielectric properties [3]. The chemical structure of the obtained polymers was characterized and confirmed by Fourier Transform Infrared Spectroscopy (FTIR) and proton resonance magnetic spectroscopy (^{1}H-RMN). Optical properties, namely transparency and refractive index were determined by UV-VIS spectroscopy and ellipsometry, respectively. The dielectric constant at optical frequencies was estimated using Maxwell relationship, recommending these materials for applications in microelectronics and biomedical fields.

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PHOSPHORESCENCE OF META-BROMBENZOPHENONE

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For the first time the crystal structure and phosphorescence spectra of meta-bromobenzophenone (3BrBP) have been measured [1]. Compared to other bromo-substituted benzophenones, the crystal of 3BrBP has several important distinctions: i) eight molecules in the elementary cell (in contrast to four in other benzophenone derivatives); ii) close and almost parallel position of phenyl rings, which can promote triplet excimer emission

Integrated phosphorescence spectra of polycrystalline 3BrBP have been measured over the temperature range 1.6 to 293 K. The spectra suffer crucial changes with varying temperature. At room temperature, very weak monomer emission is observed against the background of a very strong low-energy presumably excimer emission [2]. At 1.6 K the spectrum resembles that of benzophenone, featuring C=O stretch series with quasi-linear structures against the phonon wing. This strong dependence of the phosphorescence spectra is tentatively explained as being due to excitation-related changes in the conformation of the 3BrBP molecule.

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DIELECTRIC PROPERTIES OF LIQUID CRYSTAL E7 DOPED BY DIAMOND NANOPARTICLES

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In recent years, composite systems based on liquid crystals (LCs) and nanoparticles (NPs) have been intensively investigated. Such interest is caused by a possibility of extending the range of properties of LCs and reducing the parasitic effects typical to electro-optical devices based of liquid crystals. One of the most interesting classes of the fillers is formed by carbonaceous materials including such unique objects as carbon nanotubes (CNTs) [1, 2].

In the present work, we investigate LCs filled with nanoparticles of diamond (DNPs), which is a different allotropic form of carbon. In contrast to multiwalled CNTs with a quasi-metallic conductivity (along the tube axis), DNPs are non-conductive. At the same time, the NPs of diamond are characterized by huge values of dielectric permittivity: the dielectric constant of these particles dramatically increases during the transition from macro to nanosize (from 5.75 (macrosize) to $7*10^4$ (d ~ 4nm)) [3]. The purpose of our work is to clarify whether such NPs influence on average value of dielectric permittivity of the composite. Influence of such particles on conductivity of a liquid crystal is also investigated.

We used DNPs with an average size of 10nm obtained from Aldrich. The particles were dispersed in nematic LC E7 ($\Delta\varepsilon>0$). The E7 samples with varyous degrees of purification were utilized. The concentration of the particles, C_{DNP}, was varied in the range 0-2 wt.%. The dielectric spectra of the obtained suspensions were measured in the frequency range from 0.1 to 10^6 Hz. On the basis of these spectra were determined values of dielectric constant ε' and conductivity σ of LC bulk. Dielectric measurements were carried out for planar and homeotropically aligned layers of the suspensions at room temperature and the temperature 80°C corresponding to nematic and isotropic phase, respectively.

It is established that the distribution of DNP leads to an increase in dielectric constant ε' as well as significant change in the conductivity σ of LC E7. To explain the growth of ε' with concentrations of DNPs, two possible reasons were considered: 1) disturbance of the field director of LC in the vicinity of nanoparticles and 2) the additive effect of dielectric properties of

LC and NP. Growth of the ε'(C_{DNP}) curves for the samples stabilized in isotropic phase, as well as in the case of both planar and homeotropically aligned suspensions in nematic phase indicates the dominant role of the second mechanism. In other words, DNPs bring their dielectric properties in the LC matrix.

The character of the σ(C_{DNP}) curves depended on the purity of LC E7: for the samples based on pure E7 increase of conductivity with concentration of DNPs was detected, while for the samples with increased amount of ionic impurity the reverse trend was observed. This is due to different direction of the process of the interphase ion exchange. In the suspensions based on pure LC, desorption of ionic impurity from the surface of DNPs into the LC prevails. In turn, in the samples based on the E7 enriched with an ionic impurity, adsorption of this impurity from the E7 on the surface of DNPs dominates. Consequently, adding of DNPs allowed us to extend considerably the range of dielectric parameters of LC E7.

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THE SPECTRAL PROPERTIES AND PHOTOSTABILITY OF THE BIOMACROMOLECULES

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The ribonucleic acids, DNA and RNA, are the biomacromolecular compounds that contain the genetic information used in the development and functioning of all living organisms. The main role these compounds is the long time storage and transfer of this information. However the nature of the luminescent centers of the RNA and DNA are not clear completely until now. The electronic properties of these biomacromolecules are manifested in the optical (near biologically active ultraviolet, visual and near infrared) range and connected with the presence of the pi-electronic groups in the nucleotide cells in their chains. This gives the ground to apply the optics spectroscopy methods for the RNA / DNA electronic structure investigations. These biomacromolecules are of the type of macromolecules in which the pi-electron systems are localized in separate groups and, as the result, their energy structure determined mainly by individual properties of such groups. Taking into account the facts mentioned above the optical absorption and luminescent spectra of the biomacromolecules give the possibility: to evaluate the positions of the singlet and triplet energy levels of the biomacromolecules and to determine the centers of the electronic excitations localization in these compounds.

The present work shows the comparative investigations results of the spectral properties and photostability of the DNA, RNA macromolecules, poly- and oligonucleotides. It is examined the nucleotides in the DNA and RNA are almost independent absorbing centers. In contrast to the DNA in the RNA the complexes like AT-complex that is responsible for the phosphorescence emitting are not formed. Instead of this the main triplet electronic excitations traps in the RNA are adenosine bases. These bases are the most photostable against UV-irradiation than all other nucleotides in the DNA and RNA. The later and the fact of AT-complex photostability (in the DNA) provide the existence of the DNA/RNA self-protection mechanisms against damage caused by UV-irradiation. It was found the ribonucleotides were worse photostable comparing with correspondent deoxyribonucleotides. So, the results presented above show that the DNA is more photostable than the RNA.

PHOTOINDUCED REFRACTIVE INDEX VARIATION IN THE KDP SINGLE CRYSTALS WITH INCORPORATED ANATASE NANOPARTICLES

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Potassium dihydrogen phosphate (KDP) single crystals have found variety of applications in nonlinear optics (NLO) and optoelectronics due to their unique properties. Among them are simplicity of growing wide aperture single crystals, high laser and thermal durability with efficient ultra-fast quadric NLO response, possibility of the parametric amplification of the laser pulses in comprehensive ultra-intense laser facilities.

Dioxide titanium (TiO_2) nanocrystals were incorporated into KDP matrix in order to control the optical and NLO properties. Pure KDP and the KDP crystals with TiO_2 nanoparticles (NPs) ($10^{-5} - 10^{-3}$ wt. %) were grown by the temperature reduction method. The high resolution XRD analysis has shown that the incorporation of the NPs have no essential effect on structural perfections of the composite materials [1]. In the growth process the KDP matrix can capture the NPs between the growth layer stacks effectively forming the 1D layered macroscopic structure …$KDP:TiO_2:KDP$… with spatial period 15-20 μ. It gives a possibility to incorporate TiO_2 NPs, which NLO response can be controlled by the resonant excitation of the surface states. Indeed, TiO_2 NPs incorporated into the KDP reveal a giant cubic NLO response at 1.064 μ wavelengths [2] due to the resonance excitation of the deep defect states at the NP interface.

Experimental samples with sizes $10\times10\times0.8$ mm^3 were cut from pyramidal and prismatic growth sectors normally to the optical axis of the crystal. We have studied photoinduced variations of the absorption coefficient and of the refractive index under CW excitation at 532 nm wavelength for the different concentration of the TiO_2 NPs in the KDP matrix and different growth sectors of the crystal. It was found that the incorporation of the TiO_2 NPs changes the sign and the magnitude of refractive NLO response of the KDP crystal. Moreover, photoinduced changes of the refractive index have different singes in different growth sectors. The effect can be utilized for the phase-matching conditions optical control.

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ELECTRONIC STRUCTURE, IR AND RAMAN SPECTRA OF CAGE CLUSTERS $X_N Y_N$ BASED ON IV-IV, III-V, II-VI GROUP ELEMENTS

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The prediction of a set of cage crystal-forming clusters $X_n Y_n$ occurrence from wich zeolite-like crystals based on compounds $A^{IV}B^{IV}$, $A^{III}B^{V}$ and $A^{II}B^{VI}$ can be constructed, has been made by quantum mechanics methods. Their optimized configuration, electronic structure etc have been calculated using Hartree-Fock method RHF in the 6-31G(d) basis set. Non-monotonic dependence of the stability of cage crystal-forming clusters (cohesive energy per atom and bond lengths) on the cluster geometry and the number of atoms have been determined. IR and Raman spectra and modes of vibrations for clusters C_{2n}, $B_n N_n$ and $Si_n C_n$ (n = 12, 24) and $Zn_n O_n$, $Ga_n N_n$ (n = 12) have been calculated and analyzed [1,2].

Analysis of experimental IR spectra of samples of new phase BN («E-phase»), demonstrated that except for bands 800, 1360 cm^{-1}, which are characteristic for h-BN, additional bands appear on an area 900-1300 cm^{-1}. These bands answer by peaks in calculated IR spectra of clusters of BN on an area 950-1350 cm^{-1}. In experimental Raman spectra sharp lines on 940 and 1470 cm^{-1} are well correlated with calculated modes on 850 and 1360 cm^{-1} in spectrum of $B_{24}N_{24}$. Two satellites in area on 940 cm^{-1} can be remarked. Bands with complex description of on an area 1000-1300 cm^{-1} and sharp lines on an area 200-400 cm^{-1} answer a calculation mainly. It is found that the calculated IR and Raman spectra of cage crystal-forming clusters BN responsible experimental IR and Raman spectra of the so-called «E-phase» BN. It is set that the investigational samples of crystalline phase of BN consist of cage clusters $B_{24}N_{24}$.

The Raman spectra of synthesized products of carbon (fullerite "cubic grafite") in frequency range $50-3500$ cm$^-$ were obtained[1] in Taras Shevchenko National University in Kyiv. Comparison of these spectra and the known spectra of other carbonaceous materials rotined that next to the known characteristic bands there are new intensive bands in the range of frequencies 600-800 cm^{-1}. Relative location of these bands well correlated with the Ra-

man spectrum of carbon cage claster C_{24}, which has in this range intensive peaks of vibrations and among them characteristic peak at 708 cm^{-1}, related to the fullsymmetric vibrations of cluster, expected in theory. It is set that the investigational samples of fullerite formed from cage clusters C_{24}.

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RECENT ADVANCES IN *AB INITIO* COMPUTATIONS OF MOLECULAR ELECTRONIC EXCITATION SPECTRA

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Theoretical modelling electron excitation spectra of organic (in particular, conjugated) molecules is probably the first area in which applied quantum chemistry has shown its impressing capabilities. The famous π-electron Parizer-Parr-Pople method (PPP, developed in 1950s) and later all-valence-electron semiempirical methods had no reasonable alternatives during just a half of century. The simplest one-electron nonempirical methods for excited states, like configuration interaction singles (CIS) or time-dependent Hartree-Fock (TDHF), due to its well-established defects have a little practical value. More sophisticated and computationally demanding many-electron models, like multiconfigurational self-consistent field (MCSCF), give much more reliable results but only in case of very thorough application, being in no way a "black box" tool.

It seems that the situation changed in the last decades with the development of density functional (DFT) methods. The time-dependent DFT technique (TDDFT) was realized in all major quantum chemistry program packages. It usually moves the available functionals out of the parameterization scope, therefore emphasizing their flaws. No one of the general gradient approximation (GGA) type functionals is found to be successful enough for excited states. The new functionals of meta-GGA type [1, 2], created recently, look very promising in this area and may be recommended for practical use. Along with functionals, the interpretative schemes are being developed (for example, see [3]).

On the other hand, a few coupled cluster based methods were proposed lately for a better treatment of excited states. They are also available in quantum-chemical program packages (for instance, SAC-CI in GAUSSIAN'03 and EOM-CC in NWChem 5). Due to computational difficulties, applicability of these high-quality methods is limited now to small molecules only.

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[3]. A.V.Luzanov, O.A.Zhikol, *Int. J. Quant. Chem.* **110**, 902-24 (2010); A.V.Luzanov, O.A.Zhikol, in: *Practical Aspects of Computational Chemistry I*: *An Overview of the Last Two Decades and Current Trends*, eds. J.Leszczynski, M.Shukla, H. de Rode, Springer, 2011, in press.

PRECISE CHARACTERIZATION OF MOLECULAR IODINE HYPERFINE STRUCTURE SPECTRA NEAR 640 NM

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The accurate measurement of spectral positions of iodine hyperfine transitions in visible region is the subject of many-years studies, but still is rather important due to its usage in the laser metrology and precise laser spectroscopy.

Among the various techniques of precise measurement of hyperfine splitting in molecular iodine the laser heterodyne spectroscopy is most widely used. This technique needs the two lasers locked to the separate iodine transitions and beats are measured. This method is rather complicated and has the some limitations onto the maximum spacing of measured spectral components. We here propose the frequency-modulation technique having the intrinsic, naturally build-in scale. The precision of frequency differences measurements is near 100 kHz and potentially can be further improved. The single-laser apparatus allows provide measurement in fuul laser tuning region (for Toptica laser DL 100 the typical mode-hop free tuning range is 30-50 GHz and coarse tuning 30 – 100 nm).

The frequency-modulation spectroscopy for study of iodine hyperfine transitions near 640 nm $^{127}I_2$ R(25) 8-5 was applied. The frequency reference given by the value of the modulation frequency 12, 5 MHz as frequency marker allows to find the frequency differences between hyperfine components. A controlable frequency tuning without mode hopping was achieved in range about 30 GHz by means of the electronic module DigiLock with use of a piezoelectric actuator mounted on the external laser mirror.

The counter-propagating pump and signal beams were directed into the outer iodine cell to produce the sub_Doppler resonances of saturated absorption. The probe beam of 7 mW and the pump beam of 16 mW with beam diameter of 2 mm in a 8-cm-long iodine cell were used. The iodine vapor pressure was kept constant by keeping the cold-finger temperature within 0.001 C. Phase modulation of the laser output radiation is produced by a laser diode injection current modulation at the frequency 12.5 MHz. The hyperfine structure obtained with FM spectroscopy technique (resonances of saturated absorption) of the $^{127}I_2$ R(25) 8-5 line was studied.

The possible applications of this technique for study of $^{129}I^{127}I$ and $^{129}I_2$ iodine molecules is discussed.