Electronic Processes in Organic and Inorganic Materials (ICEPOM-12)

June 1 - 5, 2020
Kamianets-Podilskyi, Ukraine

With support of
Taras Shevchenko National University of Kyiv
Institute of Physics, NASU
Kamianets-Podilskyi National Ivan Ohiienko University

ICEPOM-12
Conference abstracts

Electronic Processes in Organic and Inorganic Materials (ICEPOM-12)

June 1 - 5, 2020
Kamianets-Podilskyi, Ukraine

With support of
Taras Shevchenko National University of Kyiv

Institute of Physics, NASU

Kamianets-Podilskyi National Ivan Ohiienko University

УДК 08
ББК 30.3

ICEPOM-12 CONFERENCE ABSTRACTS: зб. тез доповідей XII міжнародної конференції ICEPOM-12, (м.Кам’янець-Подільський, 1–5 червня 2020.) / Національна Академія Наук України, Інститут фізики НАН України, Київський національного університету імені Тараса Шевченка, Кам'янець-Подільського національного університету ім. І.Огієнка. – Кам’янець-Подільський:– 2020. – 385 с.

With support of
National Academy of Science of Ukraine, Taras Shevchenko National University of Kyiv,
Institute of Physics of NAS of Ukraine, Kamianets-Podilskyi National Ivan Ohiienko University.

Sponsored by

We wish to thank the following for their contribution to the success of this conference:

Taylor & Francis Group
an informa business

Building on two centuries' experience, **Taylor & Francis** has grown rapidly over the last two decades to become a leading international academic publisher. With offices in London, Brighton, Basingstoke and Abingdon in the UK, New York and Philadelphia in the USA and Singapore and Melbourne in the Pacific Rim, the Taylor & Francis Group publishes more than 1000 journals and around 1,800 new books each year, with a books backlist in excess of 20,000 specialist titles. Taylor & Francis Group is an Informa business (www.informa.com). Informa plc is the global information provider for the academic, professional and commercial markets.

Taylor & Francis, Inc. Molecular Crystals and Liquid Crystals

Editor-in-Chief: Mortimer M. Labes, Department of Chemistry, Temple University, 1801 North Broad Street, PA 19122 USA
Primarily fundamental in tenor, MCLC publishes original research papers of both an experimental and theoretical nature in three areas of specialization: molecular crystals (spectroscopy, energy, and charge transfer, solid state reactions, photo and radiation effects); films and composites (structure, electronic, magnetic, and optical properties, transport mechanisms); and liquid crystals (electro and magneto-optical phenomena, thermodynamics, phase transitions, structure, NMR and orientation controlled spectroscopy). In all three areas, experimental manuscripts describing both preparation and properties will be considered.

INTERNATIONAL ADVISORY COMMITTEE

M.Brodyn (Ukraine)
V. Martynyuk (Ukraine)
M. Rawiso (France)
J. Sworakowski (Poland)
L. Valkunas (Lithuania)
S.Kopylov (Ukraine)

INTERNATIONAL PROGRAM COMMITTEE

Co-Chairman: *I. Savchenko*, Taras Shevchenko National University of Kyiv, Ukraine;
e-mail: iras@univ.kiev.ua
Co-Chairman: *A. Verbitsky*, Institute of Physics, NASU, Ukraine
e-mail: avsky@iop.kiev.ua

Members

P. Skabara (UK)
J. Kowalonek (Poland)
R. Karpicz (Lithuania)
A. Pud (Ukraine)
J. Grazulevicius (Lithuania)
A. Sionkowska (Poland)
O. Aksimentyeva (Ukraine)
M. Rutkis (Latvia)
Tan Mingxiong (China)
V. Kukhtin (Ukraine)
V. Le Houerou (France)
V. Figa (Italy)
B. J. Derkowska-Zielinska (Poland)

Secretary: *A. Verbitsky*, Institute of Physics, NASU, Ukraine
e-mail: avsky@iop.kiev.ua

ORGANIZING COMMITTEE

Chairman: *N. Kutsevol*, Taras Shevchenko National University of Kyiv, Ukraine
e-mail: kutsevol@ukr.net
Vice-Chairman: *I. Konet,* Kamianets-Podilskyi National Ivan Ohiienko University

Board

D. Vyshnevsky, Taras Shevchenko National University of Kyiv, Ukraine
P.Lutsyk, Aston University, UK
A.Nych, Institute of Physics, NASU, Ukraine
A. Shydlovska, Kamianets-Podilskyi National Ivan Ohiienko University

Secretary: ***V. Ovdenko***, Taras Shevchenko National University of Kyiv, Ukraine
e-mail: valeryovdenko@gmail.com

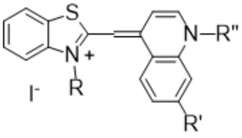
SECTION 1

ELECTRONIC PROCESSES AT INTERFACES OF ORGANIC MATERIALS WITH METALS, AS WELL AS BIOLOGICAL, ORGANIC, AND INORGANIC MEDIA

ANALOGUES OF THIAZOLE ORANGE – NEW SYNTHETIC CONDITIONS AND PHOTOPHYSICAL PROPERTIES OF LIPOPHILIC ASSYMETRIC MONOMERIC MONOMETHINE CYANINE DYES – NONCOVALENT NUCLEIC ACIDS BINDERS

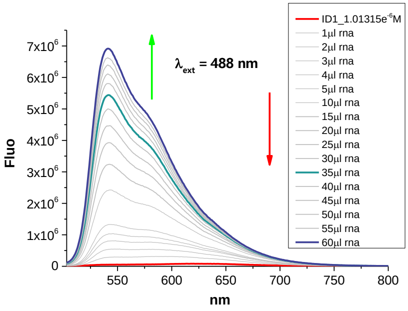
V. Videva[a,b], A. Vasilev[a], S Kitova[b], Yohan S. Georgiev[a], Kaloyan S. Kanchev[a],
Nelly Al. Stanoeva[a], Vladimir D. Petkov[a]
[a] Faculty of Chemistry and Pharmacy, Sofia University “St. Kliment Ohridski”,
1 J. Bourchier Blvd., 1164 Sofia, Bulgaria
e-mail: ohtvv@chem.uni-sofia.bg
[b] Institute of Optical Materials and Technologies “Acad. J. Malinowski”, Bulgarian Academy of Sciences, 109 Acad. G. Bontchev Str., 1113 Sofia, Bulgaria
e-mail: vvideva@iomt.bas.bg

Molecular recognition is a key factor and represents a growing research field since it allows the visualization of biomolecules as they function in their natural cellular environment. Currently, the key challenge for molecular imaging is the design and synthesis of photo stable, membrane permeable fluorescent molecules like dyes and their conjugation to biologically relevant molecules. The synthetic efforts are actually devoted to design of compounds that are based on topologically able to give rise to interactions between the carriers. Therefore, topologies that are expected to give rise fluorescent intensity enhancement in the present of DNA on/or RNA. Recently we have synthesized a series of four thiazole orange (two previously published and two novel) analogues dyes (ID) and characterized their structure in solution by NMR spectroscopy. Its ability of complex formation towards biomolecules (DNA, RNA) was investigated. All results were discussed in point of view of different aspects of their structure (number of sites donor, nature of the substitutions). In particular the incorporation of electron-withdrawing groups, such as tri-fluoromethyl substituents, significantly improve photostability of fluorophores with respect to nucleic acid labeling. The formation of stable complexes, the mechanisms of recognition allows determination the constants of associations via DNA/RNA by methods of UV-VIS Absorption and Fluorescent spectroscopy.



$R = CH_3, (CH_2)_6CH_3;$
$R' = Cl, CF_3;$
$R'' = CH_2Ph.$

ID-1-ID-4



Fluorescence $\lambda_{max\ complex}$ =539 nm

Acknowledgements. This work was performed from the students V-th grade “Pharmacy”, Faculty of Chemistry and Pharmacy, University of Sofia, during the laboratory exercises to the lecture course “Organic biomolecular probes”.

[1]. S. M. Yarmoluk, D. B. Kryvorotenko, V. B. Kovalska, *Dyes and Pigments*, **2001**, 48, 165-172.
[2]. S. M. Yarmoluk, V. B. Kovalska, I. A. Kocheshev, *Dyes and Pigments*, **2001**, 50, 21-28.
[3]. **A. Vasilev**, M. Kandinska, S. Stoyanov, S. Yordanova, D. Sucunza, J. Vaquero, O. Castaño, S. Baluschev, S. Angelova, *Beilstein J. Org. Chem.*, **2017**, 13, 2902–2914.

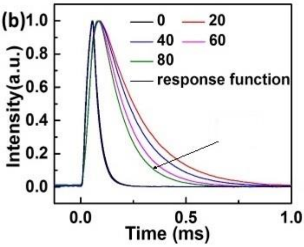
NESTED MAPPING FOR DECONVOLUTION AND FUNCTION TRANSITION

Eugen Pavlov [a], Valeriy Yashchuk [b]
[a] *Aston University, Birmingham, B4 7ET, UK,* *e-mail:* pavlovsali@gmail.com
[b] *Taras Shevchenko National University of Kyiv, Volodymyrs'ka Str., 64/13, Kyiv-01601, Ukraine,* *e-mail:* yashchukvaleriy@gmail.com

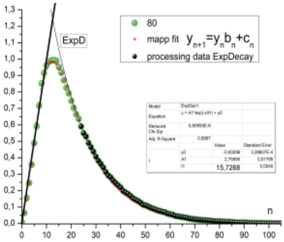
The increasing of computers power today gives the fundamental possibility of simultaneous modelling at the all scale levels. In response to this problem, recently have been developed multiscale modelling [1]. Vital to the success of this kind approach is a careful design of interphase interface [2]. The successful interface must have ability to work in the all modelling areas and provides soft transition between them. Using functions as a key element for this kind approach is problematic as a consequence of they continuity. To resolve these contradictions was using a hierarchical nested mapping system with elementary mapping, that corresponds to exponential dependency:

$$y_{n+1} = y_n b_n + c_n \quad (1)$$

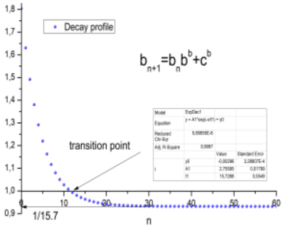
For the elementary mapping, proposed the transition scheme, which assumes the appearance of a new degree of freedom and passing to a new dependency. At the example of the excitation spectrum data [3] was shown that similar approach successfully works in the three regions: excitation pulse region, transition region and relaxation area.



Decays of PL emission data [3]



Numerical solution of (1)



Decay profile 1/ \tau=ln(b)

At the example of the excitation spectrum data [3] was shown that similar approach successfully works in the three regions: excitation pulse region, transition region and relaxation area.The numerical solution of proposed hierarchical system contains a profile of luminescence decay and allows to formulate boundaries criteria for this regions.

[1] M.Jebahi, F.Dau, J.Charles, I. Iordano, Discrete-continuum Coupling Method to Simulate Highly Dynamic Multi-scale Problems, Academic Press, 2015

[2] S.OConnell and P.Thompson, Molecular dynamics continuum hybrid computations: A tool for studying complex uid ows, Phys.Rev.E , 2014

[3] Wei Shao, Guanying Chen,Tymish Y. Ohulchanskyy, Chunhui Yang, Hans gren, and Paras N. Prasad A Core-Multiple Shell Nanostructure Enabling Concurrent Upconversion and Quantum Cutting for Photon Management,Electronic SupplementaryMaterial (ESI) for Nanoscale, 2017

PHOTOLUMINESCENCE PROPERTIES OF SIX NEW METAL-ORGANIC COMPOUNDS WITH 4,4-DIAMINODIPHENYLMETHANE LIGAND.

O.Kulikova[1] ,V.Cociu[2], M.Pliusnina[2], E.Melnic[1], L. Croitor[1], D. Chisca[1,2]
[1]*Institute of Applied Physics, Academy str., 5, Chisinau MD2028, R.Moldova.*
[2]*Tiraspol State University, Iablocikin str. 5 Chisinau MD2069, R.Moldova*
e-mail: kulikova@phys.asm.md

In recent decades, there has been great interest in the study of metal-organic supramolecular networks owing to their intriguing structural diversity and potential utility in such fields like catalysis, nonlinear optics, molecular magnetic materials, electrical conductivity and molecular recognition. Our research includes excitation and emission experiments and study of luminescent properties for a new series of Co (II), Zn (II) and Cd (II) crystalline solids that include four monomers: $[M(dadpm)_2(CH_3COO)_2(H_2O)_2]$ (M = Co(**1**); Cd(**2**)); $[Zn(dadpm)_4(H_2O)_2](NO_3)_2(H_2O)_2$ (**3**); $[Ni(dadpm)_3(dmf)(H_2O)_2][(ClO_4)_2(dadpm)(H_2O)]$ (**4**) and two one-dimensional coordination polymers: $\{[Cd(dadpm)_2(H_2O)(ClO_4)](ClO_4)\}_n$ (**5**); $\{[Cd(dadpm)_6](ClO_4)_2\}_n$ (**6**), where dadpm=4,4-diaminodiphenylmethane. Excitation of the microcrystalline samples at λ_{exc} =337 nm leads to the generation of different fluorescent emissions in the visible part of the spectrum. The maxima of the photoluminescent (PL) peaks modeling the spectrum of the dadpm ligand are observed at 1.74 eV (710 nm), 1.90 eV (650 nm), 1.95 eV (635 nm), 2.05 eV (600 nm), 2.15 eV (575 nm) and 2.5 eV (495 nm). The PL emission of the free ligand forms an intense narrow band (half-width w=0.28 eV) at hν=2.15 eV (575 nm) and three lines with a lower intensity than the main one with an order of magnitude The PL intensity of the studied complexes is several orders of magnitude weaker than those observed in PL spectra of the pure luminophore (Figure).

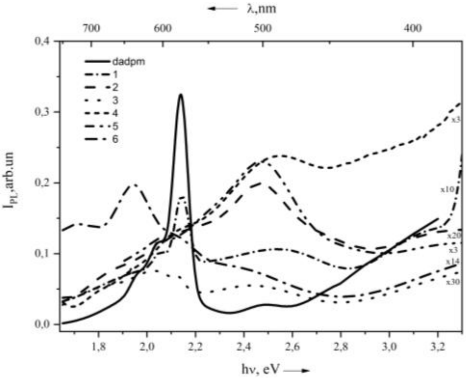


Fig. Solid-state lunimiscence emission recorded at room temperature for **dadpm** and complexes **1-6**.

The shape spectrum of free ligand (ratio of PL intensities), repeats that of complex **4**. The weakest PL intensity is observed in the Zn (II) containing complex. The emission maximum of complex **1** is shifted to the long-wavelength region. The peak has a maximum intensity at a maximum hν=1.95 eV (635 nm). In the PL spectra of all Cd (II) complexes, maximum intensity has a wide band in the short-wavelength region of the spectrum hν = 2.5 eV (495 nm), which mainly models the entire spectrum. A broad weak band is observed in the spectrum of compound **6**, at 1.9 eV (650 nm).

ANTISTOKS AND STOKS RAMAN SCATTERING IN MOLYBDENUM DISULPHIDE (MoS_2) AND GRAPHENE UNDER EXCITATION BY CONTINUOUS LASER RADIATION

Kornienko N.E., Naumenko A.P., Gubanov V.O.
Taras Shevchenko National University of Kyiv, 64/13 Volodymyrska Str., 01601 Kyiv,Ukraine
e-mail: nikkorn@univ.kiev.ua

In recent years, interest in the study of layered transition metal dichalcogenides (TMDs) MeX_2 (Me = Mo, W, etc.; X = S, Se, Te) has sharply increased in connection with their prospects for nanoelectronics, catalytic production of hydrogen, and other purposes. Raman spectra (RS) are often used to their study. However, many anomalies are observed in them: 1) strong changes in the vibrational band intensities ν_1 (E_{1g}), ν_2 (E_{2g}), ν_3 (A_{1g}) and the overtone of the longitudinal acoustic mode 2LA; 2) anomalous enhancement of the overtone bands $2\nu_2$, $2\nu_3$ and the sum tones $\nu_{2,3}$ + LA; 3) an abnormal strengthening of the anti-Stokes bands, which in some cases exceed the Stokes components; 4) a narrowing of the ν_2 and ν_3 bands with an increase in the monolayers number n_L; 5) superlinear enhancement of the $\nu_{2.3}$ bands with increasing excitation power W_L, etc. Especially a lot of anomalies recorded under excitation in resonance with excitons A, B and C, for example, for molybdenum disulfide (MoS_2) at λ_L = 632.8 and 325 nm. Some of these anomalies are also observed for graphene.

For the first time, we explain the nature of anomalies in RS of TMDs and graphene by the development of stimulated Raman scattering (SRS) processes and demonstrate this using MoS_2 and graphene as an example. It is significant that the SRS phenomenon is most pronounced in MoS_2 nanoparticles (NPs) and microcrystallites (MC) upon resonant excitation as a result of anomalous amplification of nonlinearities in nanostructures. In RS of MoS_2 (λ_L = 632.8 nm), the overtone $2\nu_3$ = 820 cm^{-1} is more than 30 times stronger than the ν_3 band, and the $2\nu_2$ + LA = 993 cm^{-1} band is more than 6 times relative to the ν_2 band. Even in the MoS_2 single crystal, the $\nu_{2.3}$ + LA bands are increased relative to $\nu_{2.3}$ by 1.15 and 1.84 times, respectively. It is known that the developed stage of SRS is characterized by the dominance of bands of the second and higher orders.

In MoS_2, we found the anti-Stokes SRS in the Stokes region, when the Stokes component ν1 = 279-286 cm^{-1} amplifies ~ 102-103 times, and the band ν_3 = 403-409 cm^{-1} is greatly attenuated. At the same time, a strong band 2LA = 463 cm^{-1} is pumped to a peak at 336 cm^{-1}. This is due to the inverse population of the state of the transverse TA mode at 124–127 cm^{-1} and the Stokes bands ν_3 and 2LA approaching resonance with exciton A (1.85 eV). In graphene, with an increase in the W_L excitation of 514.5 nm from 4 to 14 mW, the contribution of SRS to the anti-Stokes line G = 1585 cm^{-1} is more than 30%, and to the Stokes D line ~ 1350 cm-1 even more. Due to the low frequencies $\nu_{1,2,3}$ MeX_2, four-photon resonant parametric interactions play a very important role in SRS processes, which is associated with the observation of the fine linear structure of many vibrational bands. A feature of the SRS processes in MeX_2 is the interweaving of nonlinear processes involving laser pumping and nonlinear interactions of only vibrational modes in TMDs, which is confirmed by radiation at frequencies $3\nu_2$ and $3\nu_3$ in the IR spectra of the NPs and MC of MoS_2.

DETERMINATION OF THE DENSITY-OF-STATES IN OLED ORGANIC SEMICONDUCTORS USING THERMALLY STIMULATED LUMINESCENCE

Andrey Kadashchuk[a,b]
[a] *Institute of Physics of NAS of Ukraine, Prospect Nauki 46, Kyiv-03028, Ukraine*
e-mail: kadash@iop.kiev.ua
[b]*IMEC, Kapeldreef 75, Leuven, Belgium*

Density-of-States (DOS) plays a central role in controlling the charge-carrier transport in amorphous organic semiconductors. Knowledge of the DOS is also of paramount importance for modelling of charge transport in organic films and devices. Several experimental techniques were already applied for DOS probing, including UPS, inverse photoemission spectroscopy, Kelvin probe force microscopy, electrochemically gated transistor approach, as well as thermally stimulated luminescence (TSL). The TSL technique is especially suitable method for probing the DOS and extrinsic traps in luminescent organic materials, as it has been demonstrated before in our lab for different $\pi-$ and $\sigma-$conjugated polymers, molecularly doped polymers, small molecular weight oligomers, and recently, for hybrid organic-inorganic perovskite films. TSL is also of particular relevance due to it is a purely optical tool, which allows for separation of interface/contact effects and does not require good charge transport in the material. A firm theoretical background for application of TSL in disordered organic systems with hopping charge transport has been also developed, which demonstrated that the high temperature wing of the TSL curve is an exact replica of the deeper portion of the DOS distribution.

In the present work we have applied the low-temperature fractional TSL technique for determination of the DOS in a series of important OLED host materials of different polarity; namely, thin films of 4,4′-Bis(N-carbazolyl)-1,1′-biphenyl (CBP), 3,3′-Di(9H-carbazol-9-yl)-1,1′-biphenyl (mCBP), and 3′,5-di (9H-carbazol-9-yl)-[1,1′-biphenyl]-3-carbonitrile (mCBP-CN). Charge trapping in these films was found to be originated from the intrinsic localized states located within the tail of the intrinsic DOS distribution, which act as traps at sufficiently low temperatures. The main finding are the following: (i) The deep portion of experimentally observed trap distribution can be nicely approximated by a Gaussian function; analysis of the TSL data yielded the width of the DOS that agrees well with that obtained from available charge transport measurements, (ii) The DOS profile becomes significantly broader with increasing permanent dipole moments of constituting molecules, that can be quantified well by arguments based on dipolar disorder, and (ii) Interestingly, that a Gaussian distribution in CBP and mCBP films was found to be clearly followed by an exponential low-energy tail at the deepest portion of the DOS, that was theoretically predicted before.

This work has received funding from EU Horizon 2020 Program through the Marie Skłodowska-Curie ITN ‘TADF*life*’ grant (GA no. 812872).

THE STUDY OF THE CHARACTERISTICS I – V FOR THE CHALCOGENIDE GLASS COMPOSITIONS WITH SANDWICH STURUCTURE Te-$Ge_{8.33}As_{16.67}Te_{75}$ -Al, Te-$Ge_{10}As_{20}Te_{70}$-Al AND Te-$Ge_{12.5}As_{25}Te_{62.5}$-Al

A.I. Isayev, S.I. Mekhtiyeva, H.I. Mammadova

Institute of Physics named after academician G.M. Abdullayev's of Azerbaijan National Academy of Sciences, G. Javid ave 13, AZ1143 Baku, Azerbaijan,Phone:(+994 12)539-35-28, Fax: (+994 12) 5395961, Email: physics.humay@mail.ru

In this work have been studied the characteristics I–V for the chalcogenide glass compositions have sandwich structure Te-$Ge_{8.33}As_{16.67}Te_{75}$ -Al, Te-$Ge_{10}As_{20}Te_{70}$-Al and Te-$Ge_{12.5}As_{25}Te_{62.5}$-Al at the room temperature. The research shows that, the I–V characteristics of all compositions starting with an almost Ohm's law with an increase in voltage go into the region corresponding to a power law, i.e. $I \sim V^n$, where $n \approx 2$. Further is observed region where $n > 2$, which with increasing voltage also goes to the area where $n \approx 2$. Using the classical theory of injection currents [1], some parameters are determined controlling the transfer of electric charge in a wide range of applied voltage. The resistivity values of compositions were calculated from the ohmic region of I-V characteristic and using them were estimated the concentrations of equilibrium free holes according to the formula $\rho = (\varepsilon p_0 \mu)^{-1}$, where e is the elementary charge and μ -is the drift mobility of charge carriers. The mobility values were estimated using the mobility of the constituent elements [2], taking into account their percentage in the studied glass compositions. The Fermi level was determined in the band gap (F_o - E_v). By using the voltage values, which a sharp increase value of current begins (the section of the maximum filling of traps, traps filling limit - V_{TFL}) is determined the concentration of the level of adhesion, which is not filled in thermodynamic equilibrium. In our experiments have been shown that, a sharp increase in current does not occur vertically, but according to a power law ($I \sim V^n$). This fact is explained by Rose and Lampert with the assumption that the trap centers are not mono-energetic, and their densities are exponentially distributed over the energies [1,3]. Alternative explanations of this type of behavior of I – V characteristics in the TFL region were proposed by the authors of [4] with the adoption of a Gaussian distribution of defective states. The research shows that at these high values of the applied electric field ($10^3 \div 10^4$ V/cm) effects Bullet-Frenkel will inevitably affect the current transport mechanism [5]. The mechanism of this effect is the thermo-field free of charge carriers from Coulomb traps existing in the bulk of a material amplified by an electric field [6].

[1] Lampert M., Mark P., Injection currents in solids. M. Publishing House, Mir, 1973, 413 pp.
[2] Tuan T. Tran, Jennifer Wong-Leung [1] et all, Non-localized states and high hole mobility in amorphous germanium, Preprint · August 2019
[3] A. Rose, Space-Charge-Limited Currents in Solids, Phys. Rev. 97, 1538 (1955).
[4] N. F. Mott and R.W. Gurney, Electronic Processes in Ionic Crystals (Oxford University Press, London, 1940). H. T. Nicolai, M. M. Mandoc, and P.W. M. Blom, Phys.Rev. B 83, 195204 (2011)
[5] J. Frenkel, “On Pre-Breakdown Phenomena in Insulators and Electronic Semi-Conductors”, Physical Review, 54, No. 8, pp. 647-648, October 15, 1938.
[6] W. R. Harrell, “Pool-Frenkel Conduction in Silicon Dioxide Films, and Implications for Hot-Carrier Degradation in n-MOS Devices”, Doctoral Dissertation, University of Maryland, 1994

THE INFLUENCE OF TARTARIC ACID ON DPPH RADICAL SCAVENGING ACTIVITY OF VITAMIN C

Crina Vicol*, Gheorghe Duca
Institute of Chemistry, 3 Academiei str., MD-2028, Chisinau, Republic of Moldova;
**e-mail:* crina.smigon@gmail.com

Antioxidants are listed as additives in food, cosmetic and pharmaceutical products for their property to inhibit oxidation by donating an electron to the reactive species [1]. As an organic acid, ascorbic acid (AA) is, probably, the most studied antioxidant, being a good DPPH$^{\bullet}$ scavenging agent.

Tartaric acid (TA) is a preventive antioxidant, naturally occurring in grapes, and widely used in food processing for it efficiency in pH controlling, preservation, metal chelation [2], etc. When combined with primary antioxidants, organic acids are often referred to as synergists, in this case, the combined activity being greater than the sum of the individual antioxidant effects applied separately [3, 4].

For our experiments we applied the DPPH$^{\bullet}$ scavenging reaction, which is widely diffused as an easy to use method of antioxidant capacity evaluation [5]. The hydrogen atom transfer reaction from a free radical scavenger to the DPPH$^{\bullet}$ caused a decrease in absorbance at 517 nm, which was registered with a Lambda 25 UV/VIS Spectrophotometer (Perkin Elmer), using 10mm quartz cuvettes.

In order to determine the contribution of tartaric acid to the DPPH radical scavenging activity of ascorbic acid, different concentrations of both organic acids were taken. The concentration of tartaric acid varied from 0.28 mM to 270 mM, and were established according to the amount of this acid found naturally in grape and wines [6]. Various concentrations of ascorbic acid were used, and a single concentration of 0,25 mM for the free radical was taken, in order to satisfy the different molar ratios, expressed as moles of antioxidant per mole of DPPH$^{\bullet}$: 0.24, 0.36 and 0.54.

The results showed that concentrations of both organic acids are equally important. Thereby, a smaller concentration of AA in combination with a bigger TA concentration provide an increase of the antioxidant effect, which is in part due to the capacity of TA of lowering the redox potential.

[1] J. Pokorny et al., *Woodhead Pub. Ltd*, 2010, p. 380.
[2] J. A. Maga et al., *Marcel Dekker Inc.*, 1994, p. 552.
[3] R. Lo Scalzo, *Food Chem.*, 2008, vol. 107, no. 1, pp. 40–43.
[4] P. R. Quiroga et al., *Food Chem.*, 2019, vol. 277, no. July 2018, pp. 267–272.
[5] W. Brand-Williams et al., *LWT - Food Sci. Technol.*, 1995, vol. 28, no. 1, pp. 25–30.
[6] V. D. Cotea et al., *București: Ed. Acad. Rom.*, 2009, vol. 1, p. 684,

SOLITON FACILITATED LONG-RANGE ELECTRON TRANSPORT IN DONOR-POLYMER-ACCEPTOR SYSTEM

Larissa Brizhik [a],
[a] *Bogolyubov Institute for Theoretical Physics, Metrolohichna Str., 14-b, 03143, Kyiv, Ukraine*
e-mail: brizhik@bitp.kiev.ua

Recent novel applications in bioelectronics such as organic photovoltaics and fuel cell technology are based on metalorganic frameworks or structures that are complexes of electroconducting compounds or substrates and polypeptides, in which electron transport occurs on large distances [1]. In the present lecture it is shown that the long-range electron transport is possible in the system Donor – Protein – Acceptor with the formation of a soliton-like electron state in the long quasi-one-dimensional molecular chain, like protein or conducting material. Two cases are considered when the chain can be modeled as a simple one-dimensional system [2] and when such a system has an alpha-helical structure with three strands, like alpha-helical proteins [3]. Formation of the soliton in the long chain takes place due to the electron-lattice coupling resulting in the appearance of the deformational potential for the electron (polaron-like effect) [4]. The values of the parameters of the system are found when the efficiency of the long-range electron transport can reach 80% and more.

These results explain the long-range electron transport in the redox processes in living organisms, as well as the electron transport in conjugated donor-acceptor copolymer semiconductors used in micro- and nanoelectronics, in particular, in photovoltaic cells, light-emitting diodes, field-effect and thin-film organic field-effect transistors (see [5,6] and references in [2,3]).

[1] P. G. M. Mileo, K. Adil, L. Davis, et al, *J. Am. Chem. Soc.* **2018** 140, 13156.
[2] L. Brizhik, B. Piette, W. Zakrzewski, *Phys.Rev. E* **2014** 90, 052915
[3] L. Brizhik, B Jingxi Luo, B.M.A.G. Piette, W.J. Zakrzewski, *Phys. Rev. E* **2019** 100, 062205.
[4] A.S. Davydov. ***Theory of Molecular Solitons***. Reidel, Dordrecht, 1985.
[5] L. Tian, Z. Hu, X. Liu, Z. Liu, et al., *ACS Appl. Mater. Interfaces* **2019** 11, 5289.
[6] H. Zhang, S. Zhang, Y. Mao, K. Liu, et al., *Polym. Chem.* ***2017***, 8, 3255.

INFLUENCE OF SPATIAL STATIC AND DYNAMIC INHOMOGENEITIES ON THE DISTRIBUTION OF ELECTROELASTIC FIELDS AND ELECTRONIC PROCESSES IN PIEZOCERAMIC COMPOSITES

I. Lebedyeva[a], V. Yashchuk[b], O. Boryseiko [a]
[a] Faculty of Mechanics and Methematics, Taras Shevchenko National University of Kyiv. Volodymyrska str., Kyiv, 01601, Ukraine
[b] Faculty of Physics, Taras Shevchenko National University of Kyiv. Volodymyrska str., Kyiv, 01601, Ukraine
e-mail: Lebedevai@ukr.net

One of the important problems in the effective functioning of electronic devices based on piezoceramic materials is the stability of their operation, which mostly depends on the possible defects (both existing from the beginning and acquired during operation) in their structure. Cavities, heterogeneous inclusions and also cracks can be such defects. These inhomogeneities of the material bring to specific distribution of mechanical stresses that in turn, induces non-uniform distribution of electric field strengths in the piezoelectric.

In connection with the above, there is a need to state and solve electroelasticity problems for piezoceramic bodies with inhomogeneities. In this paper, three model situations are considered:

1. A piezoceramic body with an internal elliptical crack.
2. A piezoceramic body containing an external elliptical crack.
3. A piezoceramic body with a spherical cavity.

In all three cases, the coupled electroelastic field in the neighborhood of inhomogeneity for the particular case of static loading was investigated. The formulas to calculate the stress-intensity factors were obtained.

The static distribution of fields under certain conditions (for example, a crack appears and develops) can be transformed into a dynamic one. Electronic processes arising in this situation can lead to electromagnetic waves emission. On the other hand, changing of the field of mechanical stresses over time can cause the generation of acoustic waves. The registration of these waves (both electromagnetic and acoustic) enables the non-destructive control of the piezoelectric devices.

OBSERVATION OF GRAPHENE- AND DIAMOND-LIKE NANOSTRUCTURES IN MoS_2-BASEDCOMPOSITES WITH SMALL CARBON ADDITIVES

Kornienko N.E.[a], Naumenko A.P.[a], Kulikov L.M.[b]
[a]*Taras Shevchenko National University of Kyiv, 64/13 Volodymyrska Str., 01601 Kyiv,Ukraine*
[b] *Frantsevich Institute for Problems of Materials Science of NAS of Ukraine, 3, Krzhizhanovsky Str., 03142, Kyiv,Ukraine*
e-mail: nikkorn@univ.kiev.ua

The unique properties of layered nanostructures of molybdenum and tungsten disulfides (MoS_2 and WS_2) are manifested not only in the successful replacement of graphene in nanoelectronics, but also in record levels in the catalytic production of hydrogen (additives of ~ 1% MoS_2 and WS_2 increase productivity by 20-40 times) and other novel technologies. We performed a comparative study of the Raman spectra (RS) of microcrystals of natural molybdenite (~7 μm) and synthesized MoS_2 - C nanohybrids under excitations of laser radiation λ_L = 488 nm and 632.8 nm. The radiation of 632.8 nm is resonant with the exciton states A and B of MoS_2, and 488 nm is at the absorption edge of the more intense C band of MoS_2. The existence of Carbon impurities in molybdenite microcrystals and the existence of diamond- and graphite-like nanostructures in them, which are identified by vibrational bands in RS (λ_L = 632.8 nm) with Raman shifts of 1083, 1163, 1243, 1330, 1353, 1594, and 1665 cm^{-1}, are shown. A detailed identification of all observed spectral components of MoS_2 and carbon nanostructures was carried out. To reliably separate overlapping vibrational bands of graphite-like structures G (k) at the boundaries of the Brillouin zone and D bands of diamond-like structures, a new methodology has been used: with a decrease in size and disordering of diamond and graphite-like structures, the frequencies of the D bands decrease, and the frequencies G (k) bands - increase. A detailed numerical analysis of the shape of the observed D and G bands in the RS of the MoS_2-C nanohybrids, including their decomposition into composite spectral components, as well as comparison with the reference spectra of detonation nanodiamonds (~5 nm) and disordered graphite, made it possible to establish the presence of graphene-like vibrational bands (1335 – 1680 cm^{-1}) and diamond-like (1160 – 1319 cm^{-1}) nanostructures. In contrast to the known D bands at 1322 – 1326 cm^{-1} nanodiamonds, the diamond-like states observed in the MoS_2–C nanohybrids are characterized by record low frequencies of 1301 – 1309 cm^{-1}.

The complication of the spectra of the analyzed nanostructures with the appearance of additional spectral components of ~1480 cm^{-1} and 1240 – 1260 cm^{-1} as a result of doubling the size of the unit cells of MoS_2 is analyzed. It was shown that the frequencies D of the bands of diamond-like nanostructures of 1301 – 1309 cm^{-1} are independent of λ_L, in contrast to the increase in the frequencies of the G (k) bands when replacing 632.8 nm → 488 nm.

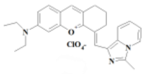
For the first time, a significant effect of 632.8 nm resonant radiation on the structure and properties of the studied MoS2-C nanohybrids was established. This is manifested in the ordering of diamond- and graphite-like structures and the decreasing of the intensity of the fundamental vibrational bands ν_1 and ν_3 of MoS_2 and the simultaneous amplification of the overtones and sum tones, as well as the observation of lines of acoustic vibrations and a strong increase in the broadband background. The strengthening of the D bands of the diamond-like structure and the ordering of the graphite structure with an increase in the carbon content in the MoS2 - C NGSs were established.

ORGANIC DYE GRAPHENE HYBRID STRUCTURES: AN AB INITIO STUDY

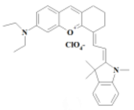
A. Navozenko[a], A. Naumenko[a], V. Gubanov[a], A. Kachkovsky[b]
[a] *Taras Shevchenko National University of Kyiv, 64/13 Volodymyrska Str., 01601 Kyiv,Ukraine*
[b] *Taras Shevchenko National University of Kyiv, 64/13 Volodymyrska Str., 01601 Kyiv,Ukraine*
e-mail: *a_naumenko@univ.kiev.ua*

Conjugated organic molecules with their collective π-electron system are extremely important for numerous applications in functional materials, due to their specific electronic and spectral properties. One of these compounds is graphene and polymethine dyes, whose composite systems have recently attracted interest from many researchers. The interaction of dye molecules with graphene-based systems is important for the development of energy stores, biological and chemical sensors and the study of molecular imaging and directed drug transport.

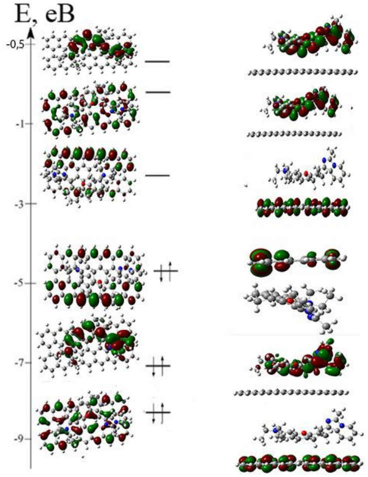
Graphene is an extended π-electron bridge system consisting of many conjugated molecules and is a suitable medium for the inclusion of a number of organic and inorganic fragments. In this work, an analysis of the model system is performed: graphene fragment and polymethine dyes



Dye 1



Dye 2



.

Figure 1
Chemical formula of dyes under study (*top*)
Energy and shape of the boundary and nearest molecular orbitals in the composite Dye 2 / graphene, calculated by TD DFT (WB97XD) for ground state geometry(*botton*)

COHERENT ANTI-STOKES RAMAN SCATTERING SPECTROSCOPY AND IMAGING OF DNA ON GRAPHENE LAYERS

Galyna Dovbeshko [a], Olena Gnatyuk [a], Andrej Dementjev [b]

[a] *Institute of Physics, National Academy of Sciences of Ukraine, 46 Nauki Ave, Kyiv 03028, Ukraine, gd@iop.kiev.ua, hrysantemka@gmail.com*
[b] *Center for Physical Sciences and Technology, Sauletekio ave. 3, Vilnius, LT-10257, Lithuania, andrej@ar.fi.lt,*

A comparative study of Raman and Coherent anti-Stokes Raman scattering (CARS) of DNA molecules deposited on single and double graphene layers and glass substrates was performed. In the DNA CARS spectra, the positions of vibrational resonances are red-shifted by 7-15 cm^{-1} in comparison with conventional Raman spectra [1] and manifestation of overtones changes spectral picture in high-frequency region in comparison with spontaneous Raman data. We demonstrate that CARS imaging can be employed for the visualization and characterization of DNA molecules deposited on graphene layers with better contrast (up to 10).

Acknowledgment. The work was supported by the projects "Smart" sensory devices of new generation based on modern materials and technologies" 2020; NATO G5291.

[1] VV Boiko, VR Romanyuk, OP Gnatyuk, OO Ilchenko, SO Karakhim, Vibrational spectra of DNA in the confined interglobular volume of photonic crystal. *Journal of Biological Physics* **2019**,44 (1), 101-116

ELECTRON TRANSPORT CHAIN IN THE LIVER BY KIDNEY DISEASE

Ferenchuk Ye., Bevzo V., Gerush I.
Higher State educational establishment of Ukraine “Bukovinian State Medical University”, Teatralna Square, 2, Chernivtsi, 58002, Ukraine
e-mail: yelena_f@ukr.net

The electron transport chain (ETC) in mitochondria is the complexes transferring electrons from electron donors to electron acceptors via redox reactions, and couples this electron transfer with the carryover of H+ ions across a cell membrane. This process creates an electrochemical proton gradient that causes ATP production. Mitochondria provide the oxidative phosphorylation and β-oxidation of fatty acids, participate in the maintaining of the cell calcium homeostasis, biosynthesis of lipids, heme, iron sulfur clusters and some amino acids etc.

Kidney diseases such as nephropathy can cause toxic damage of the liver and imbalance its mitochondrial homeostasis. Because mitochondria are considered as the main source of reactive oxygen species (ROS) which can influence intracellular signaling, regulation of cell functions and non-specific immune response, the aim of our study was to determine a state of mitochondrial ETC in the liver of rats by experimental nephropathy.

The experiment was conducted on 131 male albino rats with the body weight 0.16-0.18 kg. Experimental nephropathy was modeled by injection of a single intraperitoneal dose of folic acid (250 mg/kg, Sigma-Aldrich). Mitochondria of the liver were isolated by differential centrifugation in the isolation buffer. Significant differences between group were evaluated by using the Wilcoxon test with $P < 0.05$ considered.

The results of our experiment showed an insignificant decrease of NADH-dehydrogenase activity, succinate dehydrogenase activity decrease by 26.8% in the mitochondria of hepatocytes of rats with nephropathy on the 3 day compared to the control group. There was a decrease of succinate dehydrogenase activity by 16.7% on the 7th day of the experiment. The cause of this fact may be a violation of structural-functional organization of the I and II ETC complexes. Activities of cytochrome oxidase in the hepatocytes mitochondria of rats with nephropathy were decreased by 50% during all experimental period and it can be considered as a compensatory reaction of the organism to oxidative stress caused by nephropathy. The activity of H^+-ATPase in the hepatocytes mitochondria of rats with nephropathy was decreased by 37.5% on the 3rd experimental day and by 33% on the 7th day of the experiment. These findings suggest that the disease progress has an influence on ETC of hepatocytes and as a result on progression of oxidative stress in the organism. ROS released into the mitochondrial intermembrane space from the disordered ETC can damage mtDNA, hindering the production of mitochondrial proteins of ETC.

Taken together, folic acid-induced nephropathy exacerbates the oxidative stress and reduced energy-generating function by decreasing the enzyme activities of the mitochondria respiratory chain in the liver. Given the central role of the ETC to cellular metabolism, the study of electron flux through the chain is of fundamental importance to understanding key processes in the development of different diseases.

CHANGE OF ELECTROCHEMICAL POTENTIALS FOR DENTAL IMPLANTS SURFACE IN A PHYSIOLOGICAL SOLUTION

M.O. Vasylyev[a], V.S. Filatova[a], P.O. Guryn[b]
[a] *G. V. Kurdyumov Institute for Metal Physics of the N.A.S. of Ukraine, 36 Academician Vernadsky Boulevard, UA-03142 Kyiv, Ukraine*
[b] *Shupyk National Medical Academy of Postgraduate Education, 9 Dorohozhytska Str., Kyiv 04112, Ukraine*
e-mail: filatova@imp.kiev.ua

In the practice of metal implants installed in the oral cavity, complex corrosion processes occur, associated with the electrochemical interaction of the titanium implant surface not only with the mouth fluid, but also with blood, lymph, tissue fluid, which are active electrolytes. Therefore, despite the common viewpoint about titanium biocompatibility, it is necessary to consider the possibility of developing undesirable electrochemical processes for patients using titanium implants. In this regard, the measurement of electrode potentials is the most important task in terms of predicting the intensity of the process of electrochemical corrosion of dental prostheses in the oral cavity. The aim of this work was to study the kinetics of electrochemical potential changes in artificial saliva solution for dental titanium implants with different surface topography.

The titanium alloy BT6 mechanically polished to a mirror state was used as the model material for the study. “ImPlasa Hoechst dental implant” implants were also studied: GOTIC IMPLANT GTI and NORDIC IMPLANT NTI. In this work, an electrochemical cell for potential measurement was created, which consists of a two-electrode system, which includes a working electrode (titanium sample) and a comparison electrode (standard chlorine silver electrode) against which the potential was measured. As the electrolyte used a solution of artificial saliva (pH = 7.4). The initial surface topography and chemical composition were examined using a JSM-6490LV scanning electron microscope (JEOL, Japan) with an INCA Energy 450XT nitrogen-free energy-dispersion spectrometer.

The analysis of the data obtained for all the samples tested allowed us to obtain two critical values: the initiate time of the steady-state potential, i.e. the transition to the stage of slow passivation and the magnitude of the potential of the beginning of passivation. It was found that passivation of the NORDIC dental implant occurs most rapidly (20 min) and at a higher positive potential (+2.7 mV). More time (196 min) and less positive potential (+1.6 mV) are noted for the GOTIC implant. The BT6 titanium alloy sample did not reach the positive level of the passivation process during the study.

The differences in electrochemical potentials identified in the present work between the two types of implants are related to the different morphological conditions and chemical compositions of their surfaces due to different surface treatment methods.

SOME PECULIARITIES OF SPECTRAL PROPERTIES OF VARIOUS COMPOUNDS OF ADENINE NUCLEOTIDE AND POLYNUCLEOTIDE

Gryn D.V.[a], Yashchuk V.M.[a], Tkachuk Z.U.[b]
[a] *Taras Shevchenko National University of Kyiv, Physics faculty*
Volodymyrs'ka str. 64/13, Kyiv, 01601, Ukraine
[b] *Institute of Molecular Biology and Genetics, National Academy of Sciences of Ukraine,*
Zabolotnogo str. 150, Kyiv, 03143, Ukraine
e-mail: d.gryn@ukr.net

DNA is vitally important macromolecule and often used in various fields of biochemistry, biology and medicine.

In many experiments the DNA fluo- and phosphorescence emission is observed and investigated. It is known that adenine has the lowest triplet electronic energy level among the other bases of DNA (guanine, tymidine, cytosine), and DNA phosphorescence emission is mainly connected with adenine-tymidine (AT-) complexes emission.

In this work various compounds of adenine have been investigated, and their luminescence spectra are compared with pure DNA luminescence.

The UV-vis spectra as well as fluorescence and phosphorescence spectra of water solutions of DNA, AMP, polyA and deoxyadenosine were investigated at temperatures 300K and 77K.

Assumptions have been made about the shape and structure of investigated macromolecules, and the relationship between shape of the spectra and macromolecule structure.

COMPLEX FORMATION OF o-POPOP WITH THE ALKALINE EARTH METAL IONS IN ACETONITRILE SOLUTION: DFT AND MOLECULAR DYNAMICS SIMULATION STUDIES

Yuliia O. Gurova, Alexander D. Roshal, Alexander V. Kyrychenko
V. N. Karazin Kharkiv National University, 4 Svobody Sq., Kharkiv 61022, Ukraine
e-mail: yuliagurova8@gmail.com

Coordination of metal ions to organic fluorescence dyes induces distinct optical responses, which indicates the presence of certain metal species of interest. The development of sensors for ions has achieved particular importance for metal ions with biological and environmental interest. Organic fluorophores, which have an abnormally high Stokes shift, such as derivatives of 1,2-bis-(5-phenyl-oxazolyl-2)-benzenes (Fig. 1*a*) [1], are promising candidates for fluorescent sensing.

The formation of coordination complexes of o-POPOP with alkaline earth metal ions, such as Be^{2+}, Mg^{2+}, Ca^{2+}, and Ba^{2+}, was studied in acetonitrile solution with quantum chemical calculations and molecular dynamics (MD) simulations (Fig. 1*b*). The ground-state geometry optimization of the coordination complexes of o-POPOP was performed at the M06-2X/cc-pVDZ level. A LANL2DZ basis set and a pseudopotential were used for Me^{2+}. The all-atom MD simulations were carried out with the CHARMM27 force field.

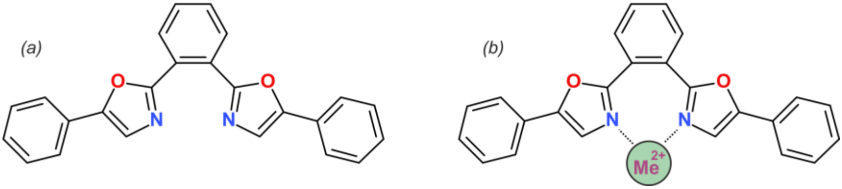


Figure 1. The structure of 1,2-bis-(5-phenyl-oxazolyl-2)-benzene (o-POPOP) (*a*) and its coordination complex with metal ions (Me^{2+}) (*b*).

We found that the formation of the complex o-POPOP:Me^{2+} with 1:1 stoichiometry alters the conformation of the fluorophore: Be^{2+} favors the flattening of o-POPOP, whereas Mg^{2+} and Ca^{2+} strongly disfavor the molecular planarity. These metal coordination-induced alterations in the structure of o-POPOP should also lead to changes in its photophysical properties, such as fluorescence Stokes shifts, which offer novel opportunities for metal ion detection in solution.

[1] A.O. Doroshenko, A.V. Kirichenko, V.G. Mitina, O.A. Ponomaryov, *J. Photochem. Photobiol. A*, **1996**, 94, 15-26.

OPTICAL SENSOR FOR DETECTING THE AMINO ACIDS CONCENTRATION IN AQUEOUS SOLUTIONS

Mykytyuk Z.M.[1], , Barylo H.I.[1], Petrina R.O.[2], Kremer I.P. [1], Ivakh M.S.[1], Prystai T.V.[1]
[1] *Electronic devices department, Lviv Polytechnic National University, S. Bandery Str., 12, Lviv-79013, Ukraine.*
E mail: zm.mykytiuk@gmail.com , mariia.s.ivakh@lpnu.ua , iryna.p.kremer@lpnu.ua
[2] *Department of Technology of Biologically Active Compounds, Pharmacy and Biotechnology, Lviv Polytechnic National University, S. Bandery Str., 12, Lviv-79013, Ukraine.*
E-mail: romanna.o.petrina@lpnu.ua

In modern pharmacology widely used a drugs and preparations based on amino acids. Detection of which in food, beverages and medicines has great importance for the technological processes control, the evaluation of raw material quality and final product. Therefore, the actual problem is to develop informative and sensitive methods for the amino acids analysis in various sites. For this purpose can be used, including optical sensors, sensing elements including a liquid crystal material [1, 2].

We studied the possibility of using cholesterol-nematic mixtures (BLO62+5CB) as an active element of optical sensors for the amino acids detection in aqueous solutions. Amino acids in aqueous solution are in the form tsviter ion. Therefore, the nature of the interaction in the system liquid crystal + amino acids aqueous solution is significantly different from the nature of the interaction in the system liquid crystal + amino acid in the crystalline form.

The spectral characteristics of the wavelength dependences of the minimum transmittance on the amino acids concentration in water were investigated. The spectral characteristics analysis shows that the linear region in comparison with the amino acid system in crystalline form increases at the dependences of the wavelengths of the minimum transmittance on the amino acids concentration in aqueous solutions. Determined range of variation in amino acids concentration in which the transfer function is linear. It is shown that the dependences of the optical transmission minimum wavelength on the amino acids concentration in water are columnar nature, namely that there is a certain amino acids concentration at which the maximum value of the minimum transmission wavelength is observed.

The hardware of the highly sensitive selective sensor is developed based on modern precision tools of leading manufacturers of electronic components, in particular Analog Device.

[1] A.N. Samoilov, S.S. Minenko, Z.M. Mykytyuk, L.N. Lisetski, Interaction of amino acids with cholesteric liquid crystals, *Spectrophotometric evidence*, *Funct. Mater.*, 26 2 (**2019**), 249-253.

[2] Z. Mykytyuk, G. Barylo, V. Virt, M. Vistak, I. Diskovskyi, Y. Rudyak, Optoelectronic Sensor Based on Liquid Crystal Substances for the Monitoring of Amino Acids, *International Scientific-Practical Connference "Problems of Infocommunications Science and Technology*", (**2018**), 177-181.

8-FORMYL-7-HYDROXYFLAVONE AS ION SENSOR. COMPLEX FORMATION WITH Mg^{2+} IONS

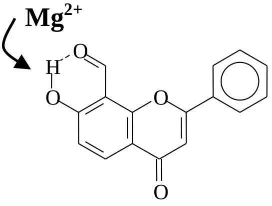
Ruslana S. Khodzhaieva, Ilia E. Serdiuk, Alexander D. Roshal
V. N. Karazin Kharkiv National University, 4 Svobody Sq., Kharkiv 61022, Ukraine
e-mail: rskhodzhaieva@gmail.com

Hydroxyflavones are known not only as strong antioxydants and convenient models for investigations of the excited-state proton transfer processes, but also as ionophores used in spectrophotometric and fluorimetric analysis of metal ions. 3- of 5-Hydroxy groups and chromone carbonyl group of the proton transfer sites can form chelate and “external” metal ion complexes that results in substantial changing in flavone absorption and emission spectra.

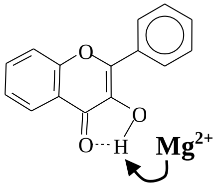
In present work we have studied spectral properties and complexation ability of a flavone containing 7-hydroxy and 8-formyl groups (FHF, see structure in Figure), and compared data obtained for Mg^{2+} complexes of FHF with those of well-known 3-hydroxyflavone.

It was found that FHF undergoes a fast proton transfer reaction in the excited state, but unlike 3-hydroxyflavone, the formed FHF phototautomer has a very low fluorescence ability probably due to long-wavelength nπ*-transition of 4-carbonyl group. Formation of the metal complex results in increase in energy of nπ*-transition, thus the appearance of Mg^{2+} in solutions leads to a sharp rise of intense fluorescence. This spectral effect allows to use FHF as Mg^{2+} ion sensor, which has better spectral characteristics than 3-hydroxyflavone. In the last case, an intense emission of 3-hydroxyflavone phototautomer masks the emission of Mg^{2+} complex, that substantially increases the detection limit of the metal ions.

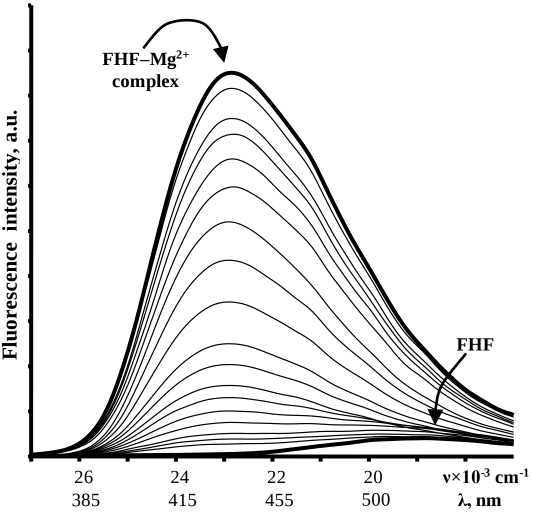
Stability of the Mg^{2+} complexes and their spectral characteristics in acetonitrile and methanol media are also studied.



8-formyl-7-hydroxyflavone



3-hydroxyflavone



FHF fluorescence spectra under complexation with Mg^{2+} ions

COMPUTER MODELING OF FRICTION OF ULTRATHIN LAYER OF CARBON DISULFIDE CONFINED BETWEEN DIAMOND SURFACES

A.V. Khomenko, D.V. Boyko, N.G. Goncharenko
Sumy State University, 2, Rimsky Korsakov Str., 40007 Sumy, Ukraine
e-mail: o.khomenko@mss.sumdu.edu.ua ; ramle2009@gmail.com

The development of wear-resistant surfaces with low friction and thin lubricating films has become an important factor in the miniaturization of moving parts in many technical devices [1, 2]. The latter include microelectromechanical systems, computer storage systems, miniature engines and so on.

The calculations were carried out for plane Couette flow geometry [3, 4], which resembles the experimental systems investigated by the surface forces apparatus. An ultrathin film of carbon disulfide was considered, bounded by two solid diamond walls with periodic boundary conditions in the plane of the plates applied to both the liquid and the surfaces. Atomically-smooth and periodic relief plates were studied. To simplify the task, the plates are considered to be absolutely rigid, and the model does not include the elasticity of the surfaces.

The behavior of the friction force, kinetic and total energies is simulated. It can be concluded from the study that the linear increase in the friction force with the load is determined not by the relief of the surfaces, but by their elasticity. This is explained by the rapid achievement of the saturation of the friction force with an increase in the load for all the models considered. Fluctuations of kinetic energy significantly increase the amplitude during the loading on the surface, this indicates an increase in the temperature of the liquid molecules. Generally, the time dependences of the friction force reflect solid-like structure of film. It is proved that increase of external load leads to a gradual transition of a film to the solid-like state. The dependences of friction force on time, external load (surface pressure), and shear force are investigated showing different rubbing modes. The dependences of shear stresses on the load obtained during the modeling show similarities with the experimental dependences for simple spherical molecules.

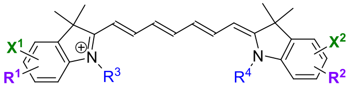
[1] E. Gnecco, E. Meyer (Eds.), *Fundamentals of Friction and Wear on the Nanoscale*, Springer – Verlag: Berlin, Heidelberg, **2007**.
[2] T. Marx, X. Shen, D. Dietzel, A. Schirmeisen, *Langmuir*, **2017**, V. 33(24), 6005.
[3] A.V. Khomenko, N.V. Prodanov, *Condens. Matter Phys.*, **2008**, V. 11, No. 4, 615.
[4] A.V. Khomenko, D.V. Boyko, M.V. Zakharov, *J. Frict. Wear*, **2018,** V. 39, No. 2, 152.

INFLUENCE OF HEAVY HALOGEN ATOMS ON SPECTRAL PROPERTIES AND QUANTUM YIELDS OF HEPTAMETHINE CYANINE DYES

Dmytro Kobzev, Olga Semenova, Olena Obukhova, Sania Khabuseva,
Olga Kolosova, Olena Stepanenko, Anatoliy Tatarets
Department of Luminescent Materials and Dyes,
SSI “Institute for Single Crystals” of the NAS of Ukraine,
60 Nauky Ave., Kharkiv, 61072, Ukraine
e-mail: kobzevua@yahoo.com

Heptamethine cyanine dyes such as Cy7, HITC and ICG are known to be used as fluorescent reporters but also sensitizers for solar cells and photodynamic therapy applications. However, the effect of bromine and iodine atoms in the terminal heterocyclic moieties on the properties of heptamethine cyanines has never been studied systematically.

In this work, a series of novel symmetrical and unsymmetrical, hydrophobic and hydrophilic heptamethine cyanine dyes BrCy and ICy which contain, respectively, bromine or iodine atoms at one or both terminal indolenine moieties was synthesized and investigated free in solutions and after binding to protein - immunoglobulin G (IgG). The spectral properties, fluorescence quantum yields, (QY(Fl)), extinction coefficients (ε), brightness (QY(Fl)*ε*D/P) photostability, photosensitizing efficiency (QY(ROS)), and phototoxicity towards red blood cells (RBC) were measured and compared to those for non-halogenated parent dyes.



BrCy: X^1, X^2 = Br
ICy: X^1, X^2 = I
R^1, R^2 = H, SO_3H;
R^3, R^4 = Me, $(CH_2)_5COOH$, $(CH_2)_4SO_3H$

The introduction of one or two bromine (BrCy) or iodine (ICy) atoms in one or both terminal heterocyclic end-groups was found to cause a red-shift of the absorption and emission bands and an increase in the sensitizing efficiency of cyanine dyes. Such a heavy atom effect was known and well investigated in the examples of different dye classes. At the same time the introduction of heavy atoms such as bromine (BrCy) and iodine (ICy) in the investigated cyanine dyes surprisingly and unexpectedly increases not only sensitizing efficiency, but also fluorescence quantum yields (QY(Fl)) and photostability, in contradiction to conventional wisdom in the art, according to which sensitizing efficiency (QY(ROS)) is increased at the cost of decreased fluorescence quantum yields.

The investigated dyes provide a unique, unexpected, and highly useful matrix of properties affording new functional advantages for reporting, diagnostics, and/or photodynamic therapy, among other applications.

MECHANISMS OF THE INTERACTION OF BOVINE SERUM ALBUMIN WITH GEMCITABINE

A.I. Lesiuk[a], O. P. Dmytrenko[a], T. O. Busko[a], O. L. Pavlenko[a]
I.P. Pundyk[a], T.M. Pinchuk-Rugal[a], M. P. Kulish[a], Chegel V.I.[b] ,
A.M. Lopatynskyi[b], Kanyuk M.I.[c], L. V. Denis[a]
[a]*Department of physics of functional materials, Physics Faculty, National Taras Shevchenko University of Kyiv, Glushkova prosp., 4, Kyiv-03039, Ukraine.*
[b]*V.Ye. Lashkaryov Institute of Semiconductor Physics of the National Academy of Sciences of Ukraine,Nauki prosp., 41, Kyiv-03028, Ukraine.*
[c]*Palladin Institute of Biochemistry of the National Academy of Sciences of Ukraine, Leontovycha str, 9, Kyiv-01601, Ukraine.*
e-mail: lesyuk.andrey@gmail.com

We investigated quantum-chemical characteristics of gemcitabine, fluorescence quenching of bovine serum albumin in water solutions with presence of gemcitabine. The static mechanism of the complex formation with moderate binding constant K_A ($\sim 4\times10^5 M^{-1}$) and number of binding sites n≈1,5 was established to take place in the solutions. Studying the energy transfer efficiency, we found that molecules of GEM locate near polar charged amino acid residues of the protein biomolecules at the average distance r=2,23 nm, R_0=2,44 nm. The calculated thermodynamic parameters demonstrate presence of both hydrogen bonds and hydrophobic interaction between the protein and ligand molecules.

Quantum-chemical analysis of gemcitabine molecule demonstrates the essential charge redistribution between the atoms, which provokes the emergence of polarity with significant dipole moment (5,4 D). Electronic configuration of the molecule indicates on the narrow gap between energetic states of the frontier orbitals HOMO and LUMO. These and neighboring molecular orbitals are located at the hexagonal ring and thus electronic transitions $\pi-\pi^*$ occur without noticeable change of their location. The largest strength of oscillator corresponds to the electronic transition with ΔE=5,55 eV, which leads to the appearance of spectral band of the optical absorption with a peak at λ_{max}= 270 nm.

STATISTICAL REPRESENTATION OF SELF-SIMILAR MODE OF ICE SURFACE PREMELTING DURING FRICTION

A.V. Khomenko[a,b], D.T. Logvinenko[a], B.N.J. Persson[b]
[a] *Sumy State University, 2, Rimsky Korsakov Str., 40007 Sumy, Ukraine*
[b] *Peter Grünberg Institut-1, Forschungszentrum-Jülich, 52425 Jülich, Germany*
e-mail: o.khomenko@mss.sumdu.edu.ua

Softening of ice surface under friction is explored in terms of the rheological model for viscoelastic matter approximation [1-4]. The nonlinear relaxation of strain and fractional feedbacks are allowed. Additive non-correlated noise associated with shear strain, stress as well as with temperature of ice surface layer, is introduced, and a phase diagram is built where the noises intensities of the stress and temperature define the domains of crystalline ice, softened ice, and two types of their mixture (stick-slip friction). Conditions are revealed under which crystalline ice and stick-slip friction proceed in the self-similar mode. Corresponding strain power-law distribution is provided by temperature fluctuations that are much larger than noise intensities of strain and stress. Since the power-type distribution is observed at minor strains it meets self-similar rubbing mode of crystalline ice surface. An analysis of the time dependences of friction force was carried out by using a fast Fourier transform. Fluctuations are detected with the spectral power density of the signal, which is inversely proportional to the frequency and demonstrates the realization of “pink” noise. It was found that the behavior of the spectrum is related to the course of the prehistory of nonequilibrium rubbing process. Research of autocorrelation function form of random fluctuations of friction force allowed to reveal the frequency characteristics of rubbing. The presence of weak correlation is shown. Constructed difference autocorrelation function of the friction force time series show power-laws confirming their self-affinity.

[1] C. Klapproth, T. Kessel, K. Wiese, B. Wies, *Tribol. Int.*, **2016**, V. 99, 169.
[2] O. Lahayne, B. Pichler, R. Reihsner, J. Eberhardsteiner, J. Suh, D. Kim, S. Nam, H. Paek, B. Lorenz, B.N.J. Persson, *Tribol. Lett.*, **2016**, V. 62(2), 1.
[3] A. Khomenko, M. Khomenko, B. Persson, K. Khomenko, *Tribol. Lett.*, **2017**, V. 65, Iss.2, Art.71.
[4] A. Khomenko, *Tribol. Lett.*, **2018**, V. 66, Iss.3, Art.82.

REASONS FOR CHANGING THE ABSORPTION SPECTRUM IN THE ASSOCIATION OF NEW METHYLENE BLUE WITH SURFACTANTS

Melnyk D. O.[a], Melnyk O. Ja.[a]
[a] *Ivano-Frankivsk national medical university, Halytska Str. 2, Ivano-Frankivsk, 76018, Ukraine*
e-mail: melnyk_dm@ukr.net

New methylene blue and other cationic dyes with a thiazine residue are used not only as drugs but also as dyes for the quantitative determination of surfactants. Their using for determination of the surfactant's concentration is related with a change in the absorption spectrum.

New methylene blue using for the detection of surfactants has several problems such as formation dimer and associates in the solution [1]. We have made quantum-chemical modelling in order to expand the scope of their use, of such structures and investigated the nature of their absorption spectra.

The results of quantum-chemical calculation show that the changing of the absorption spectrum influence both the structure of the dimer and the nature of the molecule with which associate dye. Quantum-chemical calculations of the studied structures were carried out using the semi-empirical PM6 method. These calculations show that the intensity of the first absorption band at 654 nm can sharply decrease while association with anions. Geometry optimization of this structures show that the anions are oriented towards the sulphur atom, which contributes significantly to the formation of HOMO. When surfactant associated with the anion in the energy gap is add one more energy level that change the symmetry of the frontier molecular orbitals, which leads to a decrease in the intensity of the first absorption band.

In addition to its association with anionic surfactant molecules, new methylene blue forms dimers in water. Quantum-chemical calculations of dimeric structures show that dimerization leads to a partial decrease of the intensity of the first absorption band and its displacement into the shorter wavelength region by 20 nm.

When the surfactant concentration is higher than the critical micelle concentration, there will be solubilisation of dye molecules into the micelles. Dye has not association with anions inside the micelles and the intensity of the first absorption band increase. It does not change when the concentration of surfactants increases.

Due to these properties the new methylene blue can be use as effective dye for determine both the concentration of dilute anionic surfactant solutions and the critical micelle concentration.

[1] E. Morgounova et al., Journal of Biomedical Optics, **2013**, 18, 56004

MOLECULAR DYNAMICS OF FRICTION OF METAL NANOPARTICLES ADSORBED ON GRAPHENE SHEET

A.V. Khomenko[a,b], M.V. Zakharov[a], B.N.J. Persson[b]
[a] *Sumy State University, 2, Rimsky Korsakov Str., 40007 Sumy, Ukraine*
[b] *Peter Grünberg Institut-1, Forschungszentrum-Jülich, 52425 Jülich, Germany*
e-mail: o.khomenko@mss.sumdu.edu.ua

Using classical molecular dynamics method, we investigate friction of aluminum, palladium, platinum, and cobalt nanoparticles adsorbed on a graphene layer. We study the time dependences of the total momentum of the system, the total and potential energies, the temperature, the velocity and position of the center of mass, the lateral sizes of the nanoparticle, the applied, friction, and substrate forces acting on the particle. The dependences of the substrate force on the position of the nanoparticles center of mass have been calculated for the Al nanoparticles (formed from 5 and 20 thousand atoms) and for the palladium nanoparticles (formed from 13 and 22 thousand atoms). The substrate force changes irregularly with time and coordinate, and has a sawtooth form, which is associated with stick-slip motion of the nanoparticle.

The dependences of the shear stress and friction force on the contact area have been calculated at motion of the Al nanoparticles (formed from 5-20 thousand atoms) and the palladium nanoparticles (formed from 13-22 thousand atoms). It is shown that the friction force increases approximately linearly with contact area growth. Slopes of average friction force versus contact area linear approximation at a temperature 300 K for aluminum and palladium are 0.007 nN/nm^2 and 0.015 nN/nm^2, respectively. The dependences are compared of the friction force and stress on the contact area with the use of different methods of area calculation and experimentally determined.

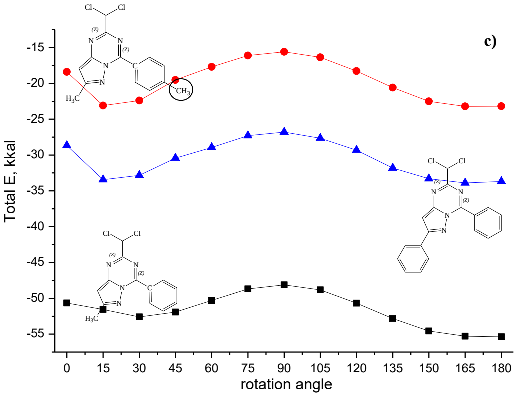
We have revealed that the friction force becomes maximal at a characteristic temperature (which ascents with increasing sliding velocity). The peaks of radial distribution function are blurred, i.e., the long-range atomic order is absent and the nanoparticles are amorphous or polycrystalline. We have observed regions of local order of atoms on the particle bottom surface. Different arrangements of the clusters on the graphene substrate cause different interaction energies which may influence the saw-like form of dependence of substrate force on time.

Calculations of motion of aluminum, palladium, and platinum nanoparticles with 10000 atoms have been performed for different temperatures and shear directions fixed by angle relatively to the axis that coincides with graphene boundary. We can conclude that at high movement velocities, the friction force is almost independent of the shear angle. Study of frictional anisotropy of nanoparticles is important for definition of the conditions for the implementation of structural lubricity (superlubricity).

ENERGY OF THE ROTATION BARRIERS PHENYL SUBSTITUENTS IN PYRAZOLO[1,5-*a*][1,3,5]TRIAZINES AS A FACTOR THE STABILIZATION OF [PHARMACOPHORE-BIOMOLECULE] COMPLEX

E. S. Veligina[a], N. V. Obernikhina[b], O. D. Kachkovsky[a], V. S. Brovarets[a]
[a]*V.P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry of the NASU,*
1, Murmanskaya str, Kyiv, 02660, Ukraine
[b]*O.O. Bogomolets National Medical University, 13 T. Shevchenko boul., 01601, Kyiv, Ukraine*
e-mail: nataliya.obernikhina@gmail.com (Nataliya V. Obernikhina)

The heterocyclic compounds with branched conjugated systems can generate the enough complementary structure with the many biopolymers, what is considered as an important condition for increasing of selectivity to potential targets. It was found that pyrazolo[1,5-*a*][1,3,5]triazines exhibit higher anticancer activity, by inhibiting cancer cell enzymes [1]. Then it could be assumed that the branched π-electronic system of the phenyl cycle should effectively participate in the mechanism of interaction of the pharmacophore with certain protein molecules.



In the interaction of pyrazolo[1,5-*a*][1,3,5]triazines with biomolecules, torsion angles of phenyl substituents play an important role for the formation and stabilization of the complex. The performed calculations give the barriers of the phenyl substituents in different positions varied appreciably. Firstly, it can be seen that the rotation barriers for phenyl introduced into the 5- and 6-membered ring of the heterocyclic “platform” are significantly different (≈6 kcal/mol). It should be noted that both barriers noticeably decrease with the simultaneous introduction of two phenyl substituents (≈3 kcal/mol), i.e., the expansion of the entire conjugated system causes a decrease in the rotation barriers of phenyl cycles. A decrease in the barrier occurs even when a weak donor methyl substituent is introduced into the p-position of the phenyl residue.

It can be assumed that a decrease in the rotation barriers of phenyl substituents will lead to a decrease in the activation energy of the interaction of pharmacophore substances with biologically active molecules (proteins, nucleic acids). Thus, the ***[Pharmacophore-Biomolecule]*** complex will form more easily and have higher stability.

[1] Sun L., Bera, H., & Chui, W. K. *Eur. J. of Med. Chem*, **2013**, 65, 1–11.

ENHANCED DNA RAMAN MODES PROBED BY SiO_2 PHOTONIC CRYSTALS

M. Olenchuk[a], T. Hanulia[a], O. Perederii[a], A. Nikolenko[b], G. Dovbeshko[a]
[a] *Institute of Physics of NASU, Kyiv, Ukraine, 03028*
[b] *Institute of Semiconductor Physics of NASU, Kyiv, Ukraine, 03028*
e-mail: m.olenchuk@yahoo.com

Nowadays, the impact of biosensitive technology is increasing. The probing of chemical and biological materials is very important because it gives an understanding of the basics of organic life. It is possible to identify various medical important biomolecules without labels with optical and electrochemical biosensors [1]. Photonic crystals (PC) can be used for optical sensing and monitoring [2]. When PC interact with light, clearly defined diffraction peaks occur, which are sensitive to changes in the size of the crystal lattice. The influence of various mechanical, optical, chemical and other factors on the investigated objects located in the volume of the PC leads to additional changes in the optical spectra.

Using the modified Stöber method a monodispersed suspensions of SiO_2 spherical particles were synthesized. Globular PC were created by sedimentation with 198 nm globules. Raman spectra of the studied samples were collected at room temperature in the backscattering geometry in single mode of Horiba Jobin-Yvon T-64000 Raman spectrometer.

Registration Raman spectra of DNA infiltrated into the pores of the PC at 488 nm excitation showed the advantages of the PC as an optical system capable of amplifying the signal. Thus, synthesized PC allowed to strengthen the bands 5-10 times. It became possible to register at an excitation power of 2.5 mW an additional 10 bands, which could not be recorded on a neutral substrate even at higher power. By increasing the excitation power by 4 times (from 2.5 mW to 10 mW) on the neutral CaF_2 substrate, we obtained the same DNA bands as the PC at 2.5 mW.

Acknowledgement: This work has been supported by NATO 985291; Development of 2D materials and "smart" sensors for medical and biological purposes 11/1 2019; Ukrainian-Polish joint research project 2018-2020 "Development of enhanced substrates based on 2D nanomaterias for fluorescent microscopy and spectroscopy: physical aspects and application"

[1] Han Sua, Xin R. Chenga, Tatsuro E., Kagan K., "Photonic crystals on copolymer film for label-free detection of DNA hybridization" *Biosensors and Bioelectronics*, **2018**, 103, p. 158–162.

[2] Xia Y., Gates B., Yin Y., Lu Y. Monodispersed colloidal spheres: Old materials with new applications. *Adv. Mater.* **2000**. V. 12. P. 693–713.

DEVELOPMENT OF AN EFFECTIVE METHOD OF MANURE CLEANING ON PIG COMPLEXES USING HIGH-VOLTAGE ELECTRIC-PULSE EQUIPMENT

A. Chmil, Y. Oliinyk
National university of life and environmental sciences of Ukraine, str. Heroyiv oborony, 12, Kyiv, 03041, Ukraine
e-mail: oljinik1202@ukr.net

The use of industrial technologies for the production of pork has increased not only the quantity of output but also the yield of manure in terms of a farm, changed the nature of the impact, increasing the risk of conditionally pathogenic microflora in the biocenosis of farms. Compared with the work of small livestock farms, the dense development of territories by livestock buildings increases the degree of pollution, and without effective methods for treating sewage can lead to an environmental disaster. In recent years, began to use the territory of former agricultural enterprises of various profiles with existing utilities to locate pig farms, near settlements. This led to non-compliance with the sizes of sanitary zones by regulatory documents. Accordingly to this problem it necessary to revise and change the regulatory values of sanitary protection zones and also to search for a new energy-efficient method of pig waste treatment.

Pig manure without bedding is a liquid substance. The development of high-voltage electro-pulse technology allows applying the phenomena of electro-pulse discharge for liquid purification. The electro-pulse discharge in liquid causes processes such as electro-hydraulic shock and cavitations initiation. The processes occurring during electro-pulse discharge in waste, adversely affect the pathogenic microflora, which allows the processing of waste faster, cheaper and without the use of chemicals.

INFRARED AND CARS SPECTROSCOPY STUDY OF MITOCHONDRIA

I. Polovyi [a], N. Piergies[b], C. Paluszkiewicz[b], A. Dementjev[c], O. Gnatyuk[a], A. Nikolenko[d], G. Dovbeshko [a]
[a] *Institute of Physics of NAS of Ukraine, Nauky ave. 46, Kyiv 03028, Ukraine*
e-mail: ipoliovy@gmail.com
[b] *The Institute of Nuclear Physics, Polish Academy of Sciences, ul. Radzikowskiego, 152, Krakow 31-342, Poland*
[c] *Center for Physical Sciences and Technology, Sauletekio ave. 3, Vilnius, LT-10257, Lithuania*
[d]*Institute of SemiconductorPhysics, NAS of Ukraine. Pr. Nauky, 41, Kyiv, UA-03028, Ukraine.*

Mitochondria have been of great interest since its very discovery. The ubiquitous roles of the organelle (from energy management to cell death initiation) require a wide range of investigation techniques. The vibrational markers of cell and mitochondria are very close in FTIR spectra; however they are slightly different in RS spectra, and therefore, spectroscopic technique is difficult for mitochondrion study. Sometimes, cytochrome c is used as a vibrational marker for mitochondria in RS spectra.

In this work, we studied the mitochondria isolated from liver according to [1] with Coherent anti-Stokes Raman scattering (CARS) spectroscopy, Raman Spectroscopy (RS) and nano-IR spectroscopy and imaging.

With nano-IR spectroscopy the infrared mapping of single mitochondrion was performed. With CARS spectroscopy unusual spectroscopic behavior was registered. Bands at 1660 cm^1 and 1460 cm^1 were local minimums in CARS spectra. Features of CARS spectrum shape connected with giant excitation of electrons was previously described [2]. Assignment of the bands in IR, Raman spectrum of mitochondrion was done and a correlation of CARS data with those for Raman data was obtained in the case of mitochondria deposited on gold support.

Acknowledgment. The work was supported by the projects "Smart" sensory devices of new generation based on modern materials and technologies" 2020; NATO G5291.

[1] Methods in cancer research. Volume VI./Edited by Harris Bush // Academic Press, New York, London, **1971**; p.160-162

[2] R A. Paddubskaya, D. Rutkauskas, R.Karpicz, G. Dovbeshko., N. Nebogatikova, Antonova I., Dementjev A.. Recognition of spatial distribution of CNT and graphene in hybrid structure by mapping with Coherent anti-Stokes Raman microscopy. Nanoscale Research Letters. 2020. Accepted.

SELF-ASSEMBLED PORPHYRIN AGGREGATES ON BIOPOLYMER SURFACE AS A PLATFORM FOR LIGHT HARVESTING AND ENERGY TRANSFER

O. Ryazanova [a], I. Voloshin [a], A. Glamazda [a], L. Dubey [b],
M. Ilchenko [b], I. Dubey [b], V. Karachevtsev [a]
[a] *B. Verkin Institute for Low Temperature Physics and Engineering of NAS of Ukraine,*
47 Nauky ave., 61103 Kharkiv, Ukraine)
[b] *Institute of Molecular Biology and Genetics of NAS of Ukraine,*
150 Zabolotnogo str., 03680 Kyiv, Ukraine
e-mail: ryazanova@ilt.kharkov.ua

Porphyrins are compounds with high biological activity and unique photophysical properties which effectively bind to nucleic acids stabilizing and changing their local structure. The presence of planar macrocyclic core in their structure determines an ability to form self-organized non-covalent multimolecular π-stacked assemblies on the surface of nucleic acids and polypeptides with strong interaction between neighboring molecules [1], which play a significant role in charge and exciton transfer and can act as artificial light-harvesting devices [2]. Two main types of molecular aggregates formed by porphyrin molecules are known, namely, *J*- and *H*-aggregates, which have different spectroscopic signatures: the Soret absorption band for porphyrin *J*-aggregates is red shifted relative to its position in the dye monomeric spectrum, while for *H*-aggregates it is blue shifted. The nature of the porphyrin aggregation is known to depend on the primary and secondary structure of the biopolymers.

The peculiarities of self-assemblies formed by water-soluble tetracationic *meso*-porphyrin, $TMPyP^{4+}$, and its tricationic derivative, $TMPyP^{3+}$, on the surface of single-stranded poly(P) and poly(A), double-stranded poly(A)·poly(U) and poly(G)·poly(C), four-stranded poly(G) at near-stoichiometric binding conditions were studied using experimental methods of absorption spectroscopy, polarized fluorescence, steady-state light scattering and resonance Raman spectroscopy as well as molecular modeling (DFT).

Acknowledgment. Authors acknowledge National Academy of Sciences of Ukraine for the financial support (Grant N 0120U100157).

[1] R.F.Pasternack, A. Giannetto, P. Pagano, E.J. Gibbs, *J. Am. Chem. Soc.*, **1991**, V. 113 (20), p. 7799–7800.
[2] L.D.A. Siebbeles, F.C. Criozema (Eds.) Charge and Exciton Transport through Molecular Wires. Wiley-VCH, Weinheim, **2011**, 500 p.

HIGH- AND LOW- ENERGY IONIZING RADIATION EFFECT ON THE BIOLOGICALLY RELEVANT AMINO ACID VALINE MOLECULE

A. Snegursky[a], E. Tamuliene[b], V. Vukstich[a], T. Snegurskaya[c], E. Romanova[a]
[a] *Institute of Electron Physics, NASU, 88017 Uzhgorod, Ukraine*
[b] *Vilnius University, Institute of Theoretical Physics and Astronomy, Lithuania*
[c] *Uzhgorod National University, 88000 Uzhgorod, Ukraine*
e-mail: snegursky.alex@gmail.com

We have studied the influence of both the high ($\geq$ 10 MeV) and low ($\leq$ 100 eV) energy ionizing radiation on the fragmentation of the valine molecule using both the experimental mass spectrometric technique and the density functional theory (DFT) approach. The results obtained demonstrate the stable structural changes in the above molecule yields under different irradiation doses (i.e. 0, 5 and 20 kGy (a, b, c, d in Fig. 1, respectively)). It has been found that the irradiation leads to the destruction of some of molecules, the degree of which depends on the irradiation dose. Figure 1 shows the mass spectra measured at the above irradiation [1].

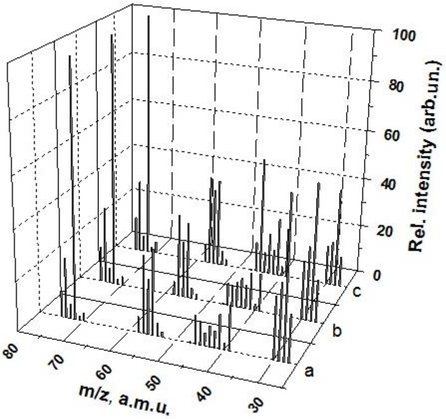


Figure 1. Mass spectra of the valine molecule irradiated at different doses.

The DFT theory approach used by us revealed that the main channel for the valine molecule dissociation under electron impact (like for most amino acids) is due to a rupture of the C–Cα bond, as a result of which the most likely process of valine-molecule dissociation is due to the neutral carboxyl group splitting off. The influence of the electric field imposition on the molecule under study has also been traced.

The analysis of the changes in the mass spectra of the valine molecules irradiated by electrons at the 5 and 20 kGy doses indicates that interaction of high-energy electrons with the valine molecule does not induce new peaks in the mass spectra measured, however, it causes significant changes in the efficiency/probability of the existing channels of this molecule dissociative ionization.

[1] V.S. Vukstich, L.G. Romanova, I.G. Megela, A.V. Papp, A.V. Snegursky, *Technical Physics Letters,* **2017**, V. 43, No. 5, pp. 416–420.

COUMARIN BASED DONOR-ACCEPTOR DYES FOR DYE-SENSITIZED SOLAR CELLS. THEORETICAL INVESTIGATION

Stepaniuk D.S.[a], Blazhynska M.M.[b] , Kalugin O.N.[a], Kovalenko S.M.[a],
Kyrychenko A.V.[a], Miannay F.-A.[b], Idrissi A.[b] , Ivanov V.V.[a]
[a]V.N. Karazin Kharkiv National University, School of Chemistry,
Svoboda sq., 4. Kharkiv, 61022, Ukraine
[b]University Lille, LASIR, Cité Scientifique, 59655, Villeneuve d'Ascq Cendex, France
e-mail: d.s.stepaniuk@gmail.com

The dye-sensitized solar cells (DSSC) attract the considerable attention of researchers due to the low cost of components and production of these devices. The main component of DSSC devices are organic π-conjugated dye with intensive light adsorption in visible region and semiconductor nanosystem. Among the different semiconductors the titanium dioxide (TiO_2) nanoclusters have attracted great interest due to low cost, environmental compatibility and significant potential ptotovoltaic applications.

In the present research, we investigated wide set of coumarin derivatives as potential systems for "dye-TiO_2" DSSC complex. Where TiO_2 in anatase form was considered. The systems include various substituents, which include not only typical donors and acceptors, but also different nature fragments in coumarin (Fig. 1).

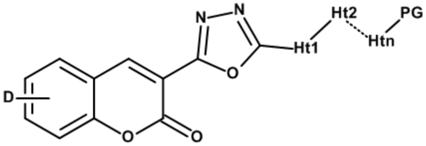


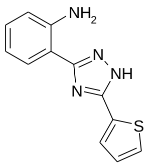
Figure 1. Structure ensembles of rings with coumarin terminal unit, which is promising for use as sensitizers for DSSC: D – substitutes affecting electro-donation of a coumarin moiety; Ht_1-Ht_2-Ht_n – π-linked heterocyclic bridge; PG – peripheral acceptor group.

To identify the most suitable compounds for DSSC elements the quantum chemistry calculations of geometrical and electronic structure of free dyes and complexes "dye–TiO_2" have been performed. Among the methods we used for calculations the semiempirical spectroscopic Pople-Pariser-Parr and full-valence AM1 approaches. Also, there were subsequent calculations by means time dependent density functional theory (TDDFT). The possibility to use different functionals (B3LYP, CAM-B3LYP, M06-2X *etc.*) in description of electronic excitations in "dye–TiO_2" complexes was discussed. Solvation effects were taken into account by classical MD simulations in explicit solvents. Comparative characteristics of excitations in free dyes and in corresponding complexes "dye–TiO_2" are presented.

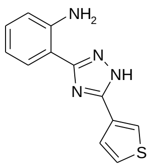
ELECTRONIC PROPERTIES OF 1,2,4-TRIAZOLE DERIVATIVES: A DFT STUDY

O. O. Pylypenko[a,b], S. I. Okovytyy[b], L. K. Sviatenko[a], T. Sergeieva[b], S. I. Kovalenko[c]
[a]*Department of General and Biological Chemistry N2, Donetsk National Medical University, 64 Komarova Str, Kropyvnytskiy, 25009 Ukraine*
[b]*Department of Organic Chemistry, Oles Honchar Dnipropetrovsk National University, 22 Kazakova Str, Dnipro, 49000 Ukraine*
[c]*Department of Pharmacy, Zaporizhzhya State Medical University, 26 Maiakovskyi avenue, Zaporizhzhia, 69035, Ukraine*
e-mail: lksv@online.ua

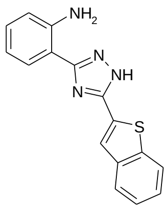
Scientists' interest in 1,2,4-triazoles is due to their use in various industries. Variation of substituents in the heterocyclic system allows the preparation of compounds with the desired properties. Therefore, the study of the relationship between the structure and properties of compounds is important in predicting their scope. In this work, a quantum chemical study of the structure, electronic properties, and energy characteristics of recently synthesized 5-substituted 3-(2-aminophenyl)-1,2,4-triazoles with substituents thiophen-2-yl, thiophen-3-yl, and benzothiophen-2-yl is carried out. Geometry optimization, molecular orbital energy calculations, and UV spectrum modeling in methanol were performed at the SMD/M06-2X/6-311++G(d,p) level using Gaussian09 program.



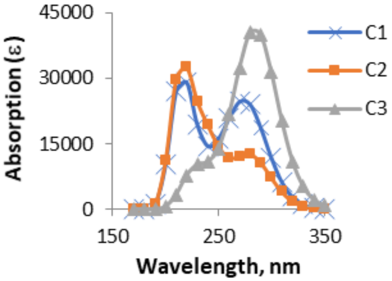
C1



C2



C3



The influence of substituents on the values of molecular orbitals energy, atomic charges, and UV spectrum is investigated. The ionization potentials, electron affinity, reduction and oxidation potentials are predicted. The reactivity indices of the compounds are analyzed.

FORMATION OF ION ASSOCIATES IN THE CARRAGEENAN - PINACYANOL SYSTEM

Iryna Syrotynska [a], Dorota Ziółkowska [b], Jan Lamkiewicz [b]
[a] *Ivano-Frankivsk National Medical University, Medical chemistry and Biochemistry Department, Halyts'ka 2, 76000 Ivano-Frankivsk, Ukraine*
[b] *UTP University of Science and Technology, Faculty of Chemical Technology and Engineering, Seminaryjna 3, 85-326 Bydgoszcz, Poland*
e-mail: irenka.933@gmail.com

Carrageenans are highly sulfated polysaccharides, widely used in food technology as gelling agents, structure stabilizers and thickeners. At least 15 different types of carrageenans are categorized based on their structural characteristics which include sulfate patterns and presence or absence of anhydrogalactose units.

Recently described methods for carrageenan and other anionic polymers quantitation are based on interaction with thiazine dye molecules[1,2]. The underlying mechanism of spectrophotometric method of anionic polymers determination is change in absorption UV-Vis spectrum of dye (e.g Methylene Blue or ortho-Toluidine Blue)[1,2] being bonded to polymer. The presented data describe interaction between exemplary anionic polymer - carrageenan and another dye - pinacyanol.

Different doses of carrageenan solution were added to the constant dose of pinacyanol dye solution. UV-Vis spectra were registered for the obtained mixtures. The most important changes in spectra shapes are observed in the visible region. With increasing amount of carrageenan, the both peaks in the dye spectrum gradually decrease because of bonding pinacyanol molecules with polymer macromolesules. At the highest doses of carrageenan, new peak appears at lower values of wavelenght. This new signal is characteristic for polymer-dye associates. Observed changes prove the metachromatic properties of pinacyanol dye. Due to low solubility of the ion associate particles, spectra of the same samples registered after sedimentation have decreased absorbance. The absorbance values at chosen wavelenghts depend strongly on carrageenan:pinacyanol ratio. Straighforward graphs were obtained for properly chosen wavelenghts, i.e. those corresponding to main peaks of the dye. For freshly prepared samples, such calibration lines are reliable in the wide range of carragenan:pinacyanol ratio. Hence, the obtained dependences between absorbance values and carrageenan content may be useful for quantitation of carrageenan.

[1] D. Ziółkowska, A. Kaniewska, J. Lamkiewicz, A. Shyichuk, *Carbohydrate Polymers*, **2017**, 165, 1–6.

[2] D. Ziółkowska, A. Shyichuk, J. Lamkiewicz, N. Kutsevol, *Molecular Crystals and Liquid Crystals*, **2018**, 672, 1, 133-141.

TOWARDS THE UNDERSTANDING OF NAD(H) COENZYME FLUORESCENCE AT AMBIENT CONDITIONS

Yuliya Terentyeva[a], Anastasiia Rashevska
[a]*Taras Shevchenko National University of Kyiv,*
64/13, Volodymyrska str., Kyiv, Ukraine, 01601
e-mail: juliater@i.ua

NAD(H) is involved in redox reactions by accepting or donating electrons and is known as fluorescent compound, if it's in reduced form. It is generally accepted, that at room temperature NAD^+, does not fluoresce, but our experiments showed that NAD^+ exhibits fluorescence in the UV region (see Fig. 1). The results of quantum chemical calculations (Gaussian 03) confirmed the presence of two emitting centers, which are the aromatic systems of nicotinamide and adenine. To optimize the geometry of the molecular structure, we used the DFT method with the PBE0 functional and the basis set of 6-311G (d, p). After the optimization has proven to be stable, ring energy was calculated to obtain the absorption spectra using the TD-DFT method with a larger basis set of 6-311G (2d, p). The calculations were carried out in an aqueous medium. To reduce the influence of statistical error in quantum mechanical calculations, caused by the imperfection of real systems and environmental factors, coefficients of 0.7 for NAD^+ and 0.8 for NADH were applied to the calculated data, which provided a better comparison of the relative position of the absorption peaks between the theoretical and experimental data. Mapping the molecular electrostatic potential over an electron isodensity surface showed that potential is larger for nicotinamide ring in NAD^+, but in the presence of hydrogen in NADH, the potential is larger for adenine ring.

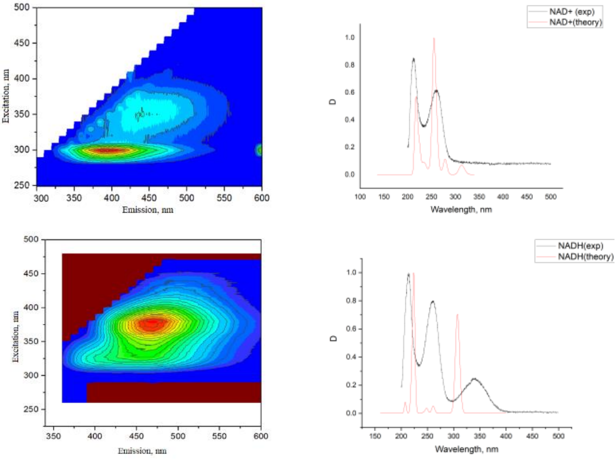


Fig. 1. Fluorescence and absorption spectra of NAD+ and NADH.

[1] https://cccbdb.nist.gov/vsfx.asp

CD SENSITIVITY OF THE MONO-CARBOXYPHENYLSULFIDE IRON(II) CLATHROCHELATES TO GLOBULAR PROTEINS

Nina Chornenka[1], Serhii Vakarov[1], Elzbieta Gumienna-Kontecka[2], Yan Voloshin[3]
Vladyslava Kovalska[4]
1 – Institute of General and Inorganic Chemistry, NASU, 32/34 Palladina Av., 03142 Kyiv
2 – University of Wroclaw, 14 F. Joliot-Curie St., 50-383 Wroclaw, Poland
3 – Institute of Organoelement Compounds RAS, 28 Vavilova St., 119991, Moscow, Russia
4 – Institute of Molecular Biology and Genetics, NASU, 150 Zabolotnogo St., 03143 Kyiv
e-mail: vakarov.s.v@gmail.com

The CD response of inherently achiral molecules induced by their assembling to chiral biomolecules, particularly proteins, are known to be sensitive to an arrangement of the hosting binding sites. In such a case deviations of induced CD (ICD) spectra may reflect both the structural alterations and the conformation transitions of proteins. Thus molecules giving ICD output upon interaction with proteins are considered as reporters potentially abile to discriminate structure variants of proteins, particularly those attributed to certain pathologies.

Recently we discovered that inherently CD silent metal complexes iron (II) clathrochelates are able to give strong induced circular dichroism (ICD) output in the range of their VIS-absrobtion bands (400-600 nm) upon such assembling with globular proteins. It was concluded that presence of ribbed carboxyphenylsulfide group is critical for the ability of clathrochelates to bind with proteins and induce the CD output on this binding.

In present work we evaluated ICD sensitivity of three constitutional isomers of mono-carboxyphenylsulfide (*ortho*-, *meta*- and *para*-) clathrochelates (**1, 2** and **3**) derivatives to globular proteins serum albumins, lysozyme, β-lactoglobulin. For all reported cage molecules, the most intensive ICD response was observed upon assembling with HSA (Fig.1).

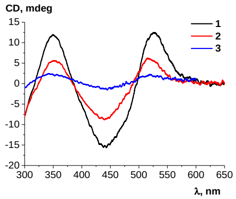


Fig.1. ICD spectra of the assemblies of HSA with the clathrochelates **1**, **2**, **3**.

Isomerism of ribbed carboxyphenylsulfide group strongly determines the intensity of ICD output of mono-carboxyphenylsulfide substituted clathrochelate upon its assembling to protein.

Conducted molecular docking has showed BSA Site 1 as the most probable place of assembling of clathrochelates **1**–**3**. Despite estimated by molecular docking energy values of the clathrochelate – BSA assembling were of the close values for **1**–**3**, the distinctions in arrangement of assembles of these clathrochelate isomers with BSA have been shown, these distinctions are suggested to cause the variation of their ICD signal intensity.

The project is funded by the EU Horizon 2020 research and innovation programme under Marie Skłodowska-Curie grant agreement № 778245.

THE SPECTRAL MANIFESTATIONS OF INTERACTION BETWEEN DNA AND METAL IONS

Gryn D.V [a]., Yashchuk V.M.[a], Ohulchanskyy T.Y.,[c] Doroshenko I.P.[a]
[a] *Taras Shevchenko National University of Kyiv, Volodymyrs'ka Str., 64/13, Kyiv-01601, Ukraine*
e-mail: Yashchukvaleriy@gmail.com
[c] *College of Optoelectronic Engineering, Shenzhen University, Shenzhen, Guangdong Province, 518060, P. R. China*

The spectral manifestations of interaction between DNA and metal (Ag, Pt, Ni, Co) ions were investigated in ultraviolet, visible and infrared spectral ranges. With this aim, optical electronic absorption, fluorescence and phosphorescence (both excitation and emission spectra) were studied, along with IR-absorption and Raman scattering spectra. It was found that while ions do not essentially influence DNA optical absorption spectrum, their presence does affect the emission spectra of DNA. In particular, presence of Co and Ni ions in DNA buffer solution causes the sharp increase in the ratio of DNA phosphorescence to fluorescence intensities, though shapes of the DNA fluorescence and phosphorescence remain unchanged.

In contrast, the presence of Ag ions in DNA solution leads to the appearance of very intensive short-wave-shifted and structured phosphorescence bands in DNA phosphorescence spectrum. It was shown that the phosphorescence emitting centers in this case are DNA adenine bases of DNA. The reasons of this observed phenomenon originated from the interaction between DNA and Ag ions will be discussed in this talkd. Finally, the effect of UV-irradiation on the spectral properties of DNA in buffer solutions in presence of metal ions will be presented.

COMPARISON OF SORBENTS FOR THE REMOVAL OF ORGANIC COMPOUNDS THAT INTERFERE WITH THE DETERMINATION OF BROMIDE IONS IN NATURAL WATERS

O.V. Zuy, Yu.I. Mazna
Dumansky Institute of Colloid and Water Chemistry of NAS of Ukraine, 42 Vernadsky Blvd, Kyiv 03142, Ukraine
e-mail: olegzuy@gmail.com

Bromide ions are a source of carcinogenic bromate ions in drinking water treated with ozone or other disinfectants. Threshold of bromides concentration, at which appreciable amounts of bromates are formed during water disinfection, is 0.04-0.05 mg/dm^3. Therefore, bromides should be monitored with adequate sensitivity in waters of different types to prevent the formation of bromates around their maximum permissible concentration (10 μg/dm^3).

In photometric and ion chromatographic methods of bromide determination the interfering effects of the dissolved organic compounds present in the waters are observed. To obtain correct, reliable results of analysis, the dissolved organic compounds are to be removed selectively from the solution so that the bromide concentration does not change therein.

The UV-VIS spectra of model organic compound - fulvic acid were recorded before and after passing through various sorbents, including Supelclean LC-18, Supelclean LC-8, SAX, Alumina-N, Amberlite XAD-2, DEAE-cellulose, Polysorb-1, Silasorb SPH C18, Silasorb SPH C8, Supelclean ENVI-18. The columns with sorbents were preconditioned first with 2 cm^3 of 96% ethanol, then with 2 cm^3 of distilled water. From 2 to 10 cm^3 of sample acidified to pH 2.0 were passed through a column, the first 10 drops of filtrate were discarded. The remaining filtrate was used to record the absorption spectra of organic matter in ultraviolet region or to perform a photometric reaction for bromide ions using standard Phenol Red method.

Experiments have shown that the most effective way to remove fulvic acids (main natural water constituents) from solution is to use Supelclean LC-18 sorbent. SAX and DEAE-cellulose sorbents effectively remove organic matter from the samples as well as a large portion of bromide ions. Polysorb-1 and XAD-2 do not remove effectively organic matter from the sample. Experiments have also shown that the loss of bromide after filtering samples containing bromide ions (0.1 mg/dm^3) and a mixture of bromide ions (0.1 mg/dm^3) with fulvic acid (20 mg/dm^3) through the sorbent Supelclean LC-18, are insignificant. The relative error of determination of bromide ions in these experiments did not exceed 20%. Acidification to pH 2.0 promotes the formation of molecular undissociated forms of organic compounds in solution that are effectively separated from bromide ions on reverse phase sorbents in the process of solid phase extraction. The Black Sea water collected near Odessa, which was contaminated by oil spills, was analyzed for bromides. The results satisfactorily match the data on total bromine obtained by the ICP-MS method, which confirms the correctness of analysis.

SECTION 2

ELECTRO-OPTIC PROCESSES IN LIQUID-CRYSTAL-BASED HETEROGENEOUS SYSTEMS

SPECTROSCOPIC STUDY OF SELF-ASSEMBLING PROCESSES IN AQUEOUS SOLUTIONS OF LYOTROPIC LIQUID CRYSTALS

I. Doroshenko[a], G. Podust[a], V. Degoda[a], M. Losytskyy[a], V. M. Yashchuk[a], O. Doroshenko[a], V. Balevicius[b]
[a] *Faculty of Physics, Taras Shevchenko National University of Kyiv. Volodymyrska str., Kyiv, 01601, Ukraine*
[b] *Institute of Chemical Physics, Vilnius University, Saulėtekio av. 9, III bld., Vilnius, LT-10222, Lithuania*
e-mail: dori11@ukr.net

Lyotropic liquid crystals represent an intersection of several challenging fields of research – supramolecular self-assembling that very often takes place at mesoscopic scale and broad variety of processes in ordered complex fluids. The spontaneous aggregation due to a combination of wide set of molecular interactions, ranging from weak Van der Waals forces to strong hydrogen bonding, media and hydrophobic effects are very important phenomena in the field of both fundamental research and technological applications such as development of new materials or new ways to treat diseases. The importance of the balance between different types of intermolecular forces for designing processes at molecular scale was reported recently [1] showing that the transfer of assembles of the lipid rafts into the surfactant-based lyotropic liquid crystals can be realized in reality.

Lyotropic chromonic liquid crystals (LCLCs) are a novel and important yet relatively poorly studied class of soft matter. The fact that LCLCs are water-based, suggests and promises a future role in biosensing for medical diagnostics. The most well-known LCLC materials are disodium cromoglycate (DSCG), also called cromolyn sodium, and 6-hydroxy-5-[(4-sulfophenyl)azo]-2-naphthalenesulfonic acid, also known as Sunset Yellow FCF (SSY) or Edicol.

Temperature and composition effects in Sunset Yellow FCF (SSY) aqueous solutions were studied by means of Raman spectroscopy passing through all phase transitions between isotropic phase (I) and chromonic phases - nematic (N) and columnar (M). It was shown that growing of SSY aggregates is accompanied by the segregation of water in the intercolumnar areas and the life time of those aggregates is 10^{-8} s or even longer [2]. Raman O–H stretching band shape shows that water confined in the intercolumnar areas behaves as in the neat substance. When the sample is heated and the transition from M phase to N phase occurs, the molecular motion of water is seen to change in a manner similar to that when water is melting.

[1] Y. S. Lee, *J. Am. Chem. Soc.*, **2017**, 139, 47, 17044-17051.

[2] K. Kristinaitytė, A. Maršalka, L. Dagys, K. Aidas, I. Doroshenko et al. *J. Phys. Chem. B*, **2018**, 122, 3047–3055.

DIELECTRIC RELAXATION AND ELECTROOPTIC EFFECTS IN FULLERENES-DOPED NEMATIC LIQUID CRYSTALS

T.D.Ibragimov, A.R.Imamaliyev, G.F.Ganizade
Institute of Physics, Azerbaijan National Academy of Sciences, 131 H.Javid Avenue, Baku, AZ1143, Azerbaijan
e-mail: tdibragimov@mail.ru

Temperature and frequency dependences of dielectric and conductivity parameters, and also electrooptic characteristics of fullerenes C_{60}-doped nematic liquid crystals 5CB and MBBA with positive and negative dielectric anisotropy, correspondingly, were studied. Firstly it is shown that fullerenes reduce clearing temperature. The real part of dielectric permittivity decreases in both liquid crystals at presence of fullerenes but the longitudinal component changes more than the transverse one. In this case, dielectric anisotropy of 5CB decreases while dielectric anisotropy of MBBA increases. A presence of fullerenes in these liquid crystals also reduces electric conductivity. The threshold voltage of Freedericksz effect increases in 5CB and it decreases for MBBA. The threshold voltage of the Carr – Helfrich electrohydrodynamic instability increases and the limiting frequency of the the Williams domain disappearance decreases for MBBA. Switching times of electrooptic effects for 5CB and MBBA decrease. Activation energy, rotation viscosity and elastic constants are determined

Experimental results are explained by location of fullerenes between liquid crystal molecules reducing their interaction. As a result, the order parameter and viscosity of the matrix decrease. Moreover, fullerenes have the traps for moving ions. Hence, the conductivity decreases and it also influences on characteristics of the Carr – Helfrich effect.

DYNAMIC CHARACTERISTICS OF THE ELECTRICALLY DRIVEN LIQUID CRYSTAL PLANARS LIGHT GUIDE

O. Chaban[1], A. Fechan[1], Y. Ilnytskyi[1,2], V. Kotsun[3], V. Yakovyna[1]
[1]*Lviv Polytechnic National University, 12 Bandera str., Lviv 79013, Ukraine*
e-mail: afechan@gmail.com
[2] *Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine,*
1 Svientsitskii Street, Lviv 79011, Ukraine
[3]*Lviv Affiliate of European University, 5 Kushevych str., Lviv, 79019, Ukraine*

In modern electronics, there is a need for active optical elements which can change their optical properties without moving elements. Such devices are perspective, since their characteristics are significantly dominated by devices with mechanical elements. Non-mechanical optical systems are smaller, more controlled and reliable. Perspective materials for creating such optical systems are electrochromic [1] and liquid crystal materials [2]. However, the use of liquid crystal materials for creation the light guide structure requires a number of problems to be solved, in particular to improve the dynamic characteristics. This requires a detailed analysis of the reorientation process of liquid crystal molecules in an external electric field.

The results of computer simulation of the reorientation process of nematic liquid crystal with negative dielectric anisotropy are presented in the paper. The simulation was performed using the GBMOLDD program. The computer simulation results were confirmed by experimental conoscopic studies obtained for the liquid crystal layer under the influence of an electric field.

The studying of the dynamic characteristics of nematic liquid crystals reorientation process in an external electric field revealed the presence of a minimum of switching-on time (formation of a light guide structure), depending on the voltage value. The obtained increase in the switching time at high (more than 50V) voltage values can be explained by a temporary decrease in the nematic order of the sample under the influence of an electric field caused by the loss of translational ordering of the nematic layer, which is determined only by the initial orientation of pretilt direction.

[1] Investigation of dry-deposited ion storage layers using various oxide particles to enhance electrochromic performance, Dahyun Choia, Minji Leea, Hyungsub, KimaWon-shik, ChubDoo-man, ChuncSung-HoonAhnb, Caroline Sunyong Leea, *Solar Energy Materials and Solar Cells,* **2018,**V. 174, pages 599-606.

[2]. Liquid crystal lenses with tunable focal length, Yi-Hsin Lin,Yu-Jen Wang &Victor Reshetnyak, *Liquid Crystals Reviews,* **2017,** V. 5, pages 111-143.

SPECTROPHOTOMETRIC STUDY OF RELATIVE CONTENT OF FLAVONOIDS IN NATURAL OBJECTS

Yu. Myagchenko, O. Tereshchenko, P.Vartik, I. Doroshenko
Faculty of Physics, Taras Shevchenko National University of Kyiv. Volodymyrska str., Kyiv, 01601, Ukraine
e-mail: myagchy@ukr.net

A method of analysis of aqueous extracts from natural objects for the presence of flavonoids by the interaction of studied samples with aluminum chloride ($AlCl_3$) has been developed and tested. Propolis was chosen as the test substance because it is a mixture of resins of many plants, pollen and the secretion of bee glands, which are the source of flavonoids [1]. Aqueous extracts of propolis were prepared with different values of oxidation-reduction potential (- 650 mV, 200 mV) and at different temperatures of extraction (20, 30, 40, 50 °C). To obtain samples with negative redox potential we used a reaction of water with magnesium, in result of which hydrogen is released.

Absorption spectra of the prepared extracts were registered using a refurbished and automated spectrophotometer SF-56 as well as Macy UV-1800PC spectrophotometer. Fluorescence spectra were measured using Cary Eclipse fluorimeter.

A comparison of absorption spectra of the prepared extracts of propolis, quercetin, rutine and commercial solutions "Propolis water extract" (produced by "Apioproduct") and "API-VI" (produced by "Phitapisvit") in pure form and with addition of aluminum chloride was made. As a result, conclusions about the possibility of analyzing substances for the presence of flavonoids were drawn.

For estimation of relative concentrations of flavonoids in the extracts a program for minimizing of functions of many variables using the Hooke - Jeeves method [2] has been developed and implemented.

[1] J.M. Sforcin, V. Bankova, *J. Ethnopharmacol.*, **2011**, 133(2), 253–260.
[2] R. Hooke, T.A. Jeeves, *Journal of the ACM*, **1961**, 8 (2), 212–229.

INFLUENCE OF MEROCYANINE DYE AGGREGATION ON SINGLE AND DOUBLE-PHOTON EXCITATION OF FLUORESCENCE IN A LIQUID CRYSTAL TEMPLATE

M. B. Malynovskyi, Yu. P. Piryatinski
Institute of Physics NAS of Ukraine, pr. Nauky 46, Kyiv, Ukraine, 03028
[a] *e-mail: malmark@ukr.net*

The optical properties of merocyanine dyes derived from malonodinitrile in a nematic liquid crystal (LC) n-pentyl-n’-cyanobiphenyl (5CB) were investigated. The LC was used as an orienting template. Since merocyanine molecules have an elongated shape, they were oriented along the LC molecules. The dye molecules might be in both molecular and aggregated forms depending on the concentration. The conformational changes in dye molecules under the influence of the LC matrix, their aggregates and related nonlinear optical properties were of our interest.

A high efficiency process of converting IR exciting radiation into visible radiation was found during the study of single- and two-photon excited luminescence. This phenomenon is associated with two-photon absorption of dye aggregates in the LC matrix and second harmonic generation. It was shown that the second harmonic generation is observed in the merocyanine dye aggregates only with certain conformational changes in its structure. The stationary and time resolved emission spectra at room and low temperatures were considered.

IDENTIFICATION AMINO ACIDS IN CALLUS BIOMASS OF PLANTS BY OPTICAL SENSOR

Petrina R.O.[a], Khomyak S.V.[a], Gubriy Z.V.[a],
Kniazieva K.S.[a], Mykytyuk Z.M.[b]
[a] *Lviv Polytechnic National University, Department of Technology of Biologically Active Substances, Pharmacy and Biotechnology, 12 Bandera str., Lviv-79013, Ukraine.*
E-mail: romanna.o.petrina@lpnu.ua
[b] *Lviv Polytechnic National University, Department of Electronic Devices,*
12 Bandera str, Lviv-79013, Ukraine.

The tissue culture method was used to preserve the biodiversity of rare and endangered medicinal plants. This is new innovation biotechnology method for obtaining of biomass of plants. Callus biomass and its extracts of *Arnica montana, Calendula officinalis, Adonis vernalis, Delphinium elatum* were obtained.

Callus biomass of there plants in medium Murasige-Skuga were obtained and impact temperature (15°C and 23°C), illumination (darkness and illumination 2000 lux) and the concentration of phytohormones in the medium on callus biomass growth were investigated. Duration of cultivation was up to 50 days, obtained from 10.8 to 23.5 g/l of dry weight. All experiments were carried out 3 times and the results were processed statistically.

The extracts callus biomass of this plants were prepared by macerating 0.5 g of the callus biomass in 50 mL of 70% ethanol for 7 days, in dark, at ambient temperature. Then, each extract was filtered through a filter paper. The filtrate was quantitatively transferred to a 100 mL volumetric flask and brought to the mark with 70% ethanol, to obtain the diluted extracts. Parts of the obtained filtrate extracts were stored at −45°C for further analyses.

Liquid cristal materials with a spiral structure, namely cholesteric liquid crystal (CLC) as a material of a sensitive element of optical sensors were used for identification of amino acids (AA) in obtained extracts of callus biomass of *Arnica montana, Calendula officinalis, Adonis vernalis, Delphinium elatum*.

Analysis of spectral characteristics showed that the dependence of the wavelengths of the minimum optical transmission from concentration of AA in callus biomass of plants contains a linear range. Therefore, this concentration range can be used to identify AA using optical sensors. Prolin,glicyne, serine, leucine, phenylalanine, glutamic acid were identificated in there extracts callus biomass.

Extracts of callus biomass of plants contain, in addition to amino acids, many substances, namely proteins, phenolic compounds, flavonoids, glycosides, terpenoids, essential oils. Using this technique for the interaction of extracts with liquid crystal, you can identify aminoacids.

SPECTRAL STUDIES OF THE COMPLEX OF ADENOSINE MONOPHOSPHATE AND D-MANNITOL

Ye. Yu. Stepanenko[1]*, V.M.Yashchuk[2], Z. Yu. Tkachuk[1]
[1]*Institute of Molecular Biology and Genetics of NASU, 150, Ac. Zabolotnogo St., Kyiv, Ukraine, 03680*
[2]*Taras Shevchenko National University of Kyiv, 64/13, Volodymyrska str., Kyiv, Ukraine, 01601*
e-mail: stepanenkojack@gmail.com

Our previous studies have shown the possibility of the formation of oligoribonucleotides (ORNs) complexes with alcohol sugars [1]. ORNs consists of sequences of ribonucleotides of monophosphates. So, we decided to investigate whether ORNs components form complexes with D-mannitol (D-M). Adenine is the major contributor to the ORNs emission spectra [2]. So, we have started studies on adenosine monophosphate (AMP).

In the course of our work, the spectral characteristics of aqueous solutions of AMP, sodium salt of AMP, and their mixtures with D-M studied. We have measured absorption, fluorescence, and excitation spectra of room temperature. The spectral dependencies of these samples also measured with heating and cooling in the temperature range 0-100 °C.

In the absorption spectra, the mixture of AMP and D-M did not make a significant difference in comparison with AMP. But in the fluorescence spectra, we obtained significant differences between the fluorescence of AMP and AMP + D-M. In particular, when excited with a wavelength of 290 nm, we have structural changes in the radiation spectrum and a significant increase in intensity several times. There were no changes in the excitation of other AMP centers after the addition of D-M.

When the AMP + D-M complex is heated, the spectrum structure does not return to the appearance of pure AMP. Heating the sample leads to a decrease in the luminescence intensity of the characteristic peak, but upon cooling, the fluorescence does not return to its original level.

In the course of our research, we found the possibility of forming dimer-like complexes between AMP and D-M. Both forms of AMP form complexes, but have different degrees of interaction.

References:

[1] Ye. Yu. Stepanenko, R. Nikolaiev, Z. Tkachuk, Spectral studies of oligoribonucleotide-based drugs, (doi:10.3390/ECMC2019-06326)

[2] V.Yu.Kudrya, V.M.Yashchuk. Tne Spectral Properties and Photostability of the DNA, RNA and Oligonucleotides // Ukr. Phys. J.- 2012.- V.57, N2.- P.187-192.

ELECTRICAL CONDUCTIVITY OF COMPOSITES BASED ON 6CB LIQUID CRYSTAL AND $(Cu_6PS_5I)_{0.5}(Cu_7PS_6)_{0.5}$ SUPERIONIC NANOPARTICLES

I.P. Studenyak[a], O.V. Kovalchuk[b,c,d], S.I. Poberezhets[c], M.M. Luchynets[a],
A.I. Pogodin[a], M. Timko[e], P. Kopčanský[e]
[a]*Uzhhorod National University, 46 Pidhirna St., 88000 Uzhhorod, Ukraine*
[b]*Kyiv National University of Technologies and Design, 2 Nemyrovycha-Danchenka Str., 01011 Kyiv, Ukraine*
[c]*Institute of Physics, 46, Nauky av., 03028 Kyiv, Ukraine*
[d]*National Technical University of Ukraine "Igor Sikorsky Polytechnic University", 37 Prospect Peremogy, 03056 Kyiv, Ukraine*
[e]*Institute of Experimental Physics, 47 Watsonova Str., 04001 Košice, Slovakia*
e-mail: studenyak@dr.com

The practical application of liquid crystals (LC) have been extended by introducing different types of non-crystalline substances, in particular, nanoparticles. Recently, we started to investigate the effect of nanoparticles of superionic conductors with argyrodite structure on the LC. The superionic conductors with argyrodite structure are characterised by high ionic conductivity and low activation energy. Due to these they are the promising materials for solid state ionics. The purpose of this paper was to investigate the influence of $(Cu_6PS_5I)_{0.5}(Cu_7PS_6)_{0.5}$ superionic nanoparticles on 6CB LC.

A polar nematic 6CB LC was used in our work. $(Cu_6PS_5I)_{0.5}(Cu_7PS_6)_{0.5}$ powders were milled with a planetary ball-mill, the maximum milling time of the powder was 30 min. Nanoparticles of $(Cu_6PS_5I)_{0.5}(Cu_7PS_6)_{0.5}$ superionic solid solution introduced into the LC had an almost spherical shape with a diameter of 250 nm. The concentration of nanoparticles of $(Cu_6PS_5I)_{0.5}(Cu_7PS_6)_{0.5}$ solid solution was 0.01, 0.05 and 0.1 wt.%. The orientation of the LC in the studied cells was planar (the long axes of the molecules were directed in a certain way parallel to the plane of the electrodes). The thickness of the measuring cells was 10 μm. Dielectric properties were studied at room temperature (293 K) in the frequency range 6-10^6 Hz using an oscilloscopic method at a voltage of a measuring signal constituting 0.2 V. Based on imaginary ε'' parts of complex dielectric permittivity the electrical conductivity was calculated.

Resulting from the experimental studies, the frequency dependences of ε' and ε'' for 6CB LC with introduced nanoparticles showed that $(Cu_6PS_5I)_{0.5}(Cu_7PS_6)_{0.5}$ nanoparticles, affect the values of ε' and ε'' of 6CB LC almost similarly as Cu_7PS_6 nanoparticles, with the exception of near-electrode processes and dipole polarization. Previous studies have shown that not only each type of superionic nanoparticles makes different influence on the electrical characteristics of the samples, but also different dependences of electrical conductivity on the concentration of nanoparticles are observed. According to the results of the research, it is established that the electrical conductivity of the 6CB LC increases non-linearly by 2 times upon introducing of the nanoparticles of solid solution $(Cu_6PS_5I)_{0.5}(Cu_7PS_6)_{0.5}$ in the whole concentration range. It should also be noted that the relative change in electrical conductivity upon introducing of $(Cu_6PS_5I)_{0.5}(Cu_7PS_6)_{0.5}$ nanoparticles is smaller than that occurring upon the introduction of Cu_6PS_5I and Cu_7PS_6 nanoparticles.

INFLUENCE OF LIGHT ON THE DIELECTRIC PROPERTIES OF A MIXTURE OF NEMATIC LIQUID CRYSTAL WITH C60 FULLERENE IMPURITIES AND MOLECULAR COMPLEXES Ni-TMTAA-TCNQ

Vovk V.E., Kovalchuk O.V.
Institute of Physics NAS of Ukraine, pr. Nauky 46, Kyiv, Ukraine, 03028
e-mail: vovk@iop.kiev.ua

Influence of light on the dielectric properties of nematic LC, such as dielectric spectra, conductivity σ and dielectric losses tg δ is of interest for investigation, which was the primary purpose of the researches in this work. This work has a small part of our works [1, 2] where we studied influence of small impurity on dielectric spectroscopy and photosensitivity of molecular composites based on nematic LC, fullerene C60 and die.

The mixture of nematic liquid crystal (6CHBT), molecules C60 with attached molecules of 1,8-diaminoctane (C60D) (1 wt.%) and molecules Ni-TMTAA-TCNQ (2 wt.%) was prepared. In previous work, we investigated the solutions of LC + fullerene C60 and LC + Ni-TMTAA-TCNQ, therefore, the purpose of this study was to investigate the variation of the dielectric parameters of these systems. The impurities were directly added to the nematic LC, after which the resulting solution was stirred mechanically and treated with ultrasound.

The research of such mixtures were carried out using the oscilloscopic method [3] in the frequency range of 10^{-1}-10^{6} Hz and temperatures range 298-333 K, also in darkness and at illumination by the introducing a Teflon film between the glass plates over the protecting electrode. Due to a low viscosity of the NLC+C60D+Ni-TMTAA-TCNQ composite, filling the cells was achieved via pressurizing this composite between the electrodes. To study the influence of light, the samples was illuminated with the focused light of halogen lamps. Measurements were carried out with planar (||) and homeotropic (⊥) orientations of molecules. The thickness of a composite layer d varied in the range of 23-25 μm. Analysis of the frequency dependences of components of complex dielectric constant, measured at illumination (ε'_l) up to those measured in darkness (ε'_d) at room temperature and after heating, was performed.

On the basis of the received data and the analysis of dielectric spectra, the mechanisms of these observed effects were offered. The conductivity σ and dielectric losses tg δ of nematic and isotropic phases at different orientations of molecules in a cell were estimated.

Keywords: dielectric properties, nematic liquid crystal, orientation of molecules LC, fullerene C60, energy of activation, dielectric loss

Reference

[1] V.E. Vovk, O.V. Kovalchuk, N. Lebovka, *Liquid Crystal*, **2012**, Vol.39, №1

[2] V.E. Vovk, O.V. Kovalchuk, T.M. Kovalchuk, *SPQEO*, **2018**, V21, №4

[3] Twarowski A.J., Albrecht A.C., *J. Chem. Phys.*,**1979**, 20, 2255

SECTION 3

THIN FILM STRUCTURES AND THEIR APPLICATION

LOCAL STRUCTURE OF $Se_{95}As_5(EuF_3)_1$, $Se_{95}Te_5(Sm)_1$ AND $Ge_{20}Sb_{20.5}Te_{51}$ CHALCOGENIDE GLASSY SEMICONDUCTOR SYSTEMS

S. N. Garibova[a, b], A.I.Isayev[a], S.I. Mekhtiyeva[a], S.U. Atayeva[a]
[a]*Institute of Physics ANAS, H.Javid ave.131, Baku AZ1143, Azerbaijan*
[b]*Khazar University, 41 Mahsati Str. AZ1096, Baku, Azerbaijan*
e-mail: sqaribova@rambler.ru

Recently, many studies have focused on the analysis of material with a phase transition, which allows a reversible phase change between stable amorphous and crystalline states [1]. In this aspect, the study of the structure of the amorphous and crystalline phases of the same material can play an important role. In this work, the local structure of the $Se_{95}As_5(EuF_3)_1$, $Se_{95}Te_5(Sm)_1$ and $Ge_{20}Sb_{20.5}Te_{51}$chalcogenide glassy semiconductors (CGS) have been studied by X-ray diffraction analysis and Raman microspectroscopy. The studies were carried out at room temperature both in bulk samples made from synthesized materials and in layers 0.5–3 μm thick, obtained by thermal evaporation on a glass substrate. The X-ray diffraction patterns consist of wide bands, which indicate the amorphous of the obtained samples. Fig. 1 shows the Raman spectra of the $Se_{95}As_5(EuF_3)_1$, $Se_{95}Te_5(Sm)_1$, $Ge_{20}Sb_{20.5}Te_{51}$ film samples (curves 1,3,4) and $Ge_{20}Sb_{20.5}Te_{51}$ bulk sample (curve 2).

The appearance of a broad maximum at the 80 cm^{-1} frequency in all samples allowed us to draw conclusions about the existence of ordering on a scale covering several coordination spheres. By analyzing the features of the Raman spectrum, taking into account the literature data, the main structural elements and chemical bonds forming the amorphous matrix of the studied CGS compositions have been determined.

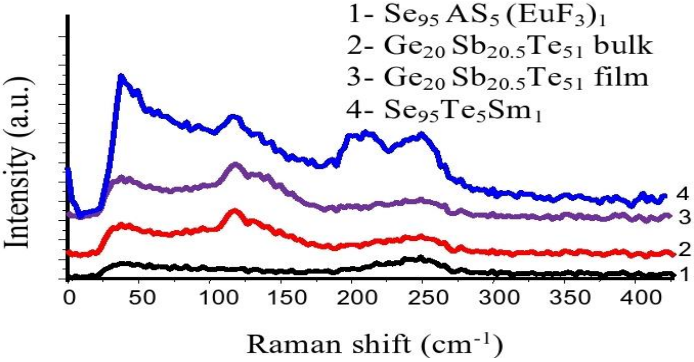


Fig.1. Raman spectra of the $Se_{95}As_5(EuF_3)_1$, $Se_{95}Te_5(Sm)_1$ and $Ge_{20}Sb_{20.5}Te_{51}$

Reference

[1] N. Yamada, E. Ohno, K. Nishiuchi, *J. Appl. Phys.***1991**, 69, issue 5, 2849–2856.

STRUCTURAL AND SPECTROSCOPIC CHARACTERISATION OF As–Se–S:Cd FILMS

Y.M. Azhniuk[a,b], V.M. Dzhagan[c], D. Solonenko[d], V.V. Lopushansky[a], V.Y. Loya[a],
V.M. Kryshenik[b], I.M. Voynarovych[a], A.V. Gomonnai[a,b], D.R.T. Zahn[d]
[a] *Institute of Electron Physics, Nat. Acad. Sci. Ukr.,*
21 Universytetska Str., Uzhhorod 88017, Ukraine
e-mail: yu.azhniuk@gmail.com
[b] *Uzhhorod National University. 46 Pidhirna Str., Uzhhorod 88000, Ukraine*
[c] *V. Lashkaryov Institute of Semiconductor Physics, Nat. Acad. Sci. Ukr.,*
45 Prospekt Nauky, Kyiv 03128, Ukraine
[d] *Semiconductor Physics, Chemnitz University of Technology, Chemnitz 09126, Germany*

Amorphous arsenic chalcogenides As_2S_3 and As_2Se_3 are well known semiconductor materials extensively studied in view of reversible or irreversible photoinduced effects leading to numerous applications. For binary As_2S_3 and As_2Se_3 films doped with group II elements laser illumination can result in the localised formation of II–VI nanocrystals due to a drastic photoenhanced diffusion in the illuminated area [1, 2]. Much less studied are As–Se–S glasses and films, especially doped with non-isovalent atoms. Here we present a study of thin (1–2 μm) As–Se–S:Cd films grown by thermal evaporation on silicate glass and Si substrates and examined by atomic force microscopy (AFM, Agilent AFM 5420), X-ray diffraction (XRD, Rigaku Smartlab), X-ray photoelectron spectroscopy (XPS, Escalab 250Xi XPS Microprobe), optical absorption spectroscopy (Cary 50), photoluminescence (PL), and micro-Raman spectroscopy (Horiba LabRAM).

The XRD and Raman studies confirmed the amorphous structure of the As–Se–S:Cd films while AFM enabled their average surface roughness and its dependence on the Cd content to be evaluated. Optical absorption spectra enable one to trace the behaviour of the film optical characteristics versus the S/Se content ratio as well as Cd concentration. The XPS data reveal a strong gradient of the Cd content decreasing with the film depth. For heavily Cd-doped As–Se–S films, the formation of $CdS_{1-x}Se_x$ crystallites on the film surface is discussed based on XRD and Raman data. In this case the chemical composition of the nanocrystals is evaluated from the Raman spectra and their average size is estimated from the PL spectra.

[1] Yu. M. Azhniuk, V.M. Dzhagan, D. Solonenko, A. Mukherjee, V. Yu. Loya, I. V. Grytsyshche, V.V. Lopushansky, A. V. Gomonnai, D. R. T. Zahn, Phys. Status Solidi B **2019**, 256, 1800298.

[2] Yu. M. Azhniuk, D. Solonenko, E. Sheremet, V. M. Dzhagan, V. Yu. Loya, I. V. Grytsyshche, S. Schulze, M. Hietschold, A. V. Gomonnai, D. R. T. Zahn, AIP Adv. **2019**, 9, 065212.

INFLUENCE OF ORGANIC AND INORGANIC ADDITIVES ON THE PROPERTIES OF NANOCELLULOSE MATERIALS

V. Barbash[a], O. Yashchenko[a], O. Alekseev[b], S. Kondratenko[b], M. Lazarenko[b], S.G. Nedilko[b], V. Scherbatskii[b], P. Teselko[b], M. Androulidaki[c], A. Manousaki[c], A. Papadopoulos[c]

[a] *National Technical University of Ukraine “Igor Sikorsky Kyiv Polytechnic Institute”, prospect Peremogy 37, Kyiv, Ukraine*
[b] *Taras Shevchenko National University of Kyiv, 64/13 Volodymyrska str., 01601 Kyiv, Ukraine*
[c] *Institute of Electronic Structure & Laser (IESL) of Foundation for Research & Technology Hellas (FORTH), Heraklion 711 10 Crete, Greece*
e-mail: v.barbash@kpi.ua

Cellulose as the raw material is the most abundant polymer on earth and various products can be made on the cellulose base. The cellulose fibrils can be obtained from various plants; thus the characteristics of the products depend on the raw material source and procedure of fibrils preparation. Cellulose materials composed of the nanoscale fibrils, so called nanocellulose (NC), draw great attention as they are lightweight, electrically conductive, nontoxic, optically transparent in the crystalline form, etc. Besides, it can be produced in large quantities in a cost-effective manner by mechanical, chemical, and fermentative methods [1]. Due to the abundant bonds between cellulose molecules as prepared nanocellulose has a tendency to form bundles, clusters or aggregates. Especially the property to be self-assembled is revealed under drying of the NC gels. That is why, properties of the solid NC depend on the type and morphology of formed clusters (aggregates) and on the structure of solid substrates, too.

It is obvious; a knowledge of the mechanisms of the NC fibrils binding is of large importance for developments of new NC based materials. Aimed to study the mechanisms we made and have studied the sets of the NC samples as liquid and in the form of the solid films. NC was extracted from different non-wood plant materials. The procedure of the NC synthesis was described in details recently [2]. The films of the noted NCs deposited on the glass, quartz and silicon substrates. Interaction between NCs fibrils was modified by means of incorporation of some additive such as oxide micro/nanoparticles, graphene oxide, and carbon nanotubes.

The non-destructive methods: XRD, viscosymetry, densitomety, scanning force and scanning electron as well as optical microscopy, were used to characterize morpho;ogy and structure of prepared nanocellulose samples. Examples of the application of the obtained nanocellulosic materials with organic and inorganic additives in optoelectronics are considered.

1. Ping Lu, You-Lo Hsieh, Carbohydrate Polymers, 2010, 82, 329–336
2. V.A. Barbash, O.V. Yashchenko, Appl. Nanoscience, 2020, doi:10.1007/s13204-019-01242-8

ELLIPSOMETRY OF NANOSTRUCTURED LAYERS

E. Bortchagovsky[a]
[a] *V. Lashkarev Institute of Semiconductor Physics of NAS of Ukraine,*
pr.Nauki 41, Kyiv 03028, Ukraine
e-mail: bortch@yahoo.com

Ellipsometry is well-known to investigate optical properties of surfaces and films. Composites are usually nanostructured heterogeneous objects, which macroscopic properties are usually described in the frame of so-called Effective-Medium Approximation (EMA) [1]. Different EMA models describe averaged properties of a composite on the base of properties of the constituting materials and rather minor information about topology of the composite giving rather robust estimations.

However, the case of nanostructured films and layers of nanoparticles has the peculiarity as such systems approach two-dimensional distribution of constituting elements. It results in the anisotropy of interactions in such films making them effectively anisotropic [2]. The same reason does not allow to apply the Lorentz sphere formalism for the fields averaging in the heterogeneous nanostructure what produces deviation of the optical properties of such a structure from results given by standard 3D models of effective-medium approximation.

This talk discusses features of optical properties of two-dimensional nanostructured layers with examples of the deficiencies of standard EMA models in the description of such films as well as ellipsometric investigations of both random and ordered structures of nanoparticles on a surface.

[1] A.H. Sihvola, Electromagnetic mixing formulas and applications, IEE electromagnetic waves series vol.47, (The Institution of Engineering and Technology, London, 1999).
[2] B.N.J. Persson, J. de Physique (Suppl.), 1983, vol.44, p.C10-409-C10-419.

ELECTROPHYSICAL PROPERTIES CARBON-DOPED THIN FILM IRON

V.O. Burlakov, O. V Filatov, O.E. Pogorelov
[a] *G. V. Kurdyumov Institute for Metal Physics, N.A.S. of Ukraine,*
36 Academician Vernadsky Blvd., UA-03142 Kyiv, Ukraine
e-mail: odinpwnzpacan@gmail.com

The electrophysical properties of the MTJ system Fe \ MgO \ Fe in the presence of carbon in one of the ferromagnet / dielectric interfaces were studied in [1]. As a result, on the I – V characteristics of the MTJ system, the authors found a region with negative differential resistance. This is typical of a tunnel diode.

To establish the nature of semiconductor properties of a carbon doped MTJ system, we studied the interaction of a nanofilm of pure iron and carbon doped iron with p- and n-type semiconductors. Metal-semiconductor contacts were made, which could turn out to be a non-rectifying ohmic contact and a rectifying contact, called the Schottky barrier [2]. Two types of semiconductor substrates were used in the experiment: KEF — monocrystalline silicon doped with phosphorus with n-type conductivity and KDB — monocrystalline silicon doped with boron with p-type conductivity. The contact pads with a thickness of 100 nm and a diameter of 2 mm made of pure iron and carbon-doped iron were sprayed by the electron-beam method in the VUP-5 setup.

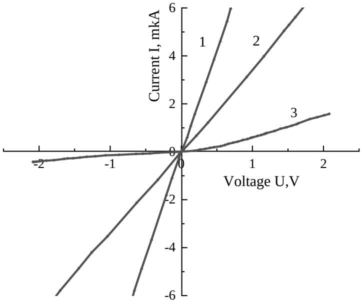


Figure 1. I – V characteristics of the studied contacts. Line 1- contacts of Fe and Fe + C on a p-type semiconductor substrate. Line 2 - both Fe contacts on an n-type substrate. Line 3 - exponential dependence for Fe and Fe + C contacts on an n-type substrate. The first two correspond to a non-rectifying ohmic contact, the third correspond to a rectifying contact characteristic of a Schottky diode.

The obtained results indicate that doping with carbon increases the work function in the Fe nanofilm, i.e. the Fermi level is below the Fermi level of the semiconductor. As a result, the ordinary ohmic contact characteristic of pure Fe on a semiconductor after doping turned into a rectifying metal-semiconductor contact. These results complement the understanding of the nature of the appearance of negative differential resistance obtained in the MTJ system when one of the iron layers is doped with carbon.

References:

[1] A. Pogorelov, A. Filatov, Ye. Pogoryelov. Negative differential resistance in magnetic tunnel junction systems, *Physica Status Solidi* (b), January 2014, pp 172 – 177, https://doi.org/10.1002/pssb.201349258

[2] J. Lutz, H. Schlangenotto, U. Scheuermann, R. De Doncke. Schottky Diodes, *Semiconductor Power Devices*, Springer, Heidelberg, 2011, pp 271-293.

OPTICAL FUNCTIONS of HEAVY DOPED ZnO:Al THIN FILMS

V. Dzikovskyi[a], O. Bovgyra[a], M. Kovalenko[a], A. Kashuba[b], H. Ilchuk[b], R. Petrus[b], I. Semkiv[b]

[a]*Faculty of Physics, Ivan Franko National University of Lviv, 8a, Kyrylo and Mefodiy St.,*
Lviv, UA–79005, Ukraine
e-mail: viktor.dzikovskyy@lnu.edu.ua
[b]*Department of General Physics, Lviv Polytechnic National University, 12, S. Bandera Str.,*
Lviv-79013, Ukraine

Zinc oxide (ZnO) has recently become the object of increasing attention due to its potential applications in optoelectronic devices, transparent conductive oxide (TCO) thin films, and spintronics devices. For the design and implementation of ZnO-based devices, one of the most effective approaches is doping. This issue is particularly important for the use of ZnO as a TCO, which necessarily involves the doping of group III trivalent elements. It is known that ZnO doped with Sn, In, Ga and Al impurities to improve the electrical and optical properties for use in transparent electronic devices. Impurity doping of ZnO is also a good method for the realization of band gap engineering.

Undoped and doped ZnO thin films have been prepared by a variety of thin film deposition techniques among which magnetron sputtering and sol-gel method most widely used. Simultaneously with experimental study methods of ZnO there is an intensive development of theoretical approaches to the investigation of the basic properties of this material for deeper understanding of electronic and optical properties in such pure and doped ZnO materials.

In this study, we apply electronic band-structure calculations to investigate the optical properties of Al-doped ZnO thin films with different impurity concentration within density functional theory (DFT). All calculations in this work are performed with the generalized gradient approximation (GGA) to DFT in the form of Perdew-Burke-Ernzerhof (PBE) and with the GGA+U extension to it. To reproduce various concentrations of Al, we considered 3×3×3, 3×3×2, and 2×2×2 supercells, corresponding to content impurity of 1.85, 2.75, and 6.25 at.%, respectively. Firstly, we accomplished geometry optimization of undoped ZnO, further one Zn atom is substituted with one Al atom for all supercells and geometry relaxation was repeated. Calculation results shows the fundamental band gap of Al-doped decreases, and the Fermi level shifts to the conduction band, which implies the appearance of an optical band gap, which expand with increases of Al content.

Using electronic band-structure for all exploring objects optical functions were calculated in order to explain the main mechanisms that contribute to the optical response of such heavily doped thin films. Comparison between theory and experiment implies a strong blueshift in dielectric-function spectra with an increase of Al content that is considerably higher than the Burstein-Moss shift predicted for the given Al concentrations.

ABSORPTION SPECTRA OF A LAYER OF METALLIC ELLIPSOIDAL NANOPARTICLES ON A SURFACE SUPPORTING SURFACE PLASMON

E.G. Bortchagovsky, Yu.V. Demydenko
V.Lashkariov Institute of semiconductor NAS of Ukraine, Nauki ave.45, 03028 Kyiv, Ukraine
e-mail: bortch@yahoo.com

Both plasmonic nanoparticles and surfaces supporting surface plasmon are widely used as modern label-free optical biosensors because of their sensitivity to tiny change of local dielectric function at the surface. However, their combination is not yet investigated in details in spite of it can enhance the sensitivity and tune it to the desired spectral range.

It is known that interacting electromagnetic modes like localized and surface plasmons in the system of nanoparticles deposited on a metal surface hybridize and split [1]. Moreover, even for spherical particles with degenerated localized mode deposition on surface results in lifting that degeneracy and creation of two separated modes along and across the surface. Both modes hybridize with the surface plasmon. However, as any other passive film, layer of nanoparticles also shifts the dispersion of the surface plasmon as the position of nanoparticle resonances can be tuned beside of used material by their shape, size and concentration on the surface [2].

This work is devoted to the theoretical modeling of optical properties of the system with ellipsoidal nanoparticles deposited on the surface supporting surface plasmon. Analysis of the system is based on the conception of effective susceptibility for nanostructured systems [3].

It was found that, for the fixed-incident angle in Kretschmann configuration with the internal reflection, very distinguishable peaks exist in the absorption spectra which are directly connected with excitations of collective electromagnetic modes in the system. Some of the peaks originate from localized plasmons of nanoparticles which are connected with charge oscillations in-plane and out-plane in a single ellipsoidal particle; one is connected with an excitation of the surface plasmon-polariton on the surface of a substrate. Position of all of them is sensitive to the change of the particle concentration in a layer what opens the door for the construction of tunable sensors working in desired spectral range. Additionally, those peaks have different sensitivity to analytes allowing to choose optimal parameters of a sensor.

---

[1] E. Bortchagovsky, *J. Vac. Sci. Technol. B*, **2020**, v.38, 013603-1-5.

[2] E. Bortchagovsky, Yu. Demydenko, in Springer Proceedings in Physics v.210, “*Nanooptics, Nanophotonics, Nanostructures, and Their Applications*”, O. Fesenko, L. Yatsenko (eds.), **2018**, 243-263.

[3] V. Lozovski, *J. Comput. Theor. Nanosci.*, **2010**, v.7, 7-17.

THE KEY ROLE OF THE NiS ELECTRODE/ELECTROLYTE INTERFACE IN LITHIUM ACCUMULATORS

R. Apostolova[a], E. Shembel[a], B. Markovsky[b], D. Aurbach[b]
[a]SHEI Ukrainian State University of Chemical Technology,
*Gagarina ave. 8, Dnipro, Ukraine, 49005, *e-mail:* apostolova.rd@gmail.com
[b]Department of Chemistry, Bar-Ilan University, Ramat Gan, Israel, 52900

Nickel sulfides are used as an electrode material for lithium batteries (LB). A number of nickel sulfides were synthesized using various technological methods. The possibility of obtaining thin-layer NiS_x–electrodes by electrolysis for miniature LB has been shown [1]. The electrochemical behavior of these electrodes depends much on the composition of the non-aqueous electrolyte. We present the results of a study of a thin-layer electrochemically prepared on stainless steel NiS electrodes in redox reactions with lithium in non-aqueous lithium perchlorate electrolytes based on a solvent of 1,3-dioxolane (DOL), as well as in a mixture of solvents DOL and tetrahydrofuran (THF). Synthesized sulfide is assigned to the hexagonal phase (space group P63/mm) with lattice parameters a=3.416 Ǻ, c=5.230 Ǻ and peak positions corresponding to NiS (JCPDS 75–0613). The surface of the NiS electrode presents granular aggregates with grain size of 25 to 50 nm. The average discharge capacity of NiS electrodes in the electrolyte with DOL (300–320 mAh/g) after 14-fold charge-discharge cycling decreases to ≤ 190 mAh/g. Identification of the reasons of the drop in discharge capacity was facilitated by the analysis of changes in the surface morphology of NiS electrodes. These changes manifest themselves in the formation of a thick surface film on these electrodes. Additional information on changes in the chemistry of the electrode/electrolyte interface was obtained by comparing the FTIR spectra of NiS electrodes: After a 14-fold discharge of the NiS electrode in the spectral region of 1200–600 cm^{-1}, the intensity of the bands assigned to surface impurities increases presumably because of the electrochemical interaction of nickel sulfide with an electrolyte with the possible formation of a surface film that impedes the electrode processes. An analysis of FTIR spectra revealed reasonable spectral stability of the region that characterizes the vibration of bonds in NiS. We have established that metal-sulfides deposited on stainless steel in non-aqueous environment can be the initiators of the corrosion processes of the base [2]. Anodic dissolution of the base occurs in the corrosion galvanic metal-sulfide/iron pair. In this case, the corrosive effects of the base can contribute to weakening the adhesion of the metal sulfide to the base, leading to a decrease in the discharge capacity of the battery.

The initial discharge capacity of the NiS electrode in a binary solvent electrolyte (DOL, THF, 1 mol/L $LiClO_4$) reaches 525–550 mAh/g. The reversible capacity of the NiS electrode for more than 50 discharge-charge cycles is maintained at 400 mAh/g with a discharge of up to 1.1 V ($i_{discharge}$=50 μA/cm^2). The reversible capacity of NiS electrodes as anodes in lithium-ion batteries can reach more than 500 mAh/g. In this report, we demonstrate the optimal conditions of charge-discharge cycling of NiS electrodes in a binary solvent electrolyte. Obviously, the presence of a THF solvent in it changes the mechanism of the surface film formation on NiS.

References: 1. R.D. Apostolova, E.M. Shembel. Thin-layer produced electrolytically metal sulfides and metal oxides of transition metals for lithium power sources. Monograph, Dnipro, LIRA 2019, 264 p. 2. D.A. Shifler, P.J. Moran, J. Kruger *Electrochim. Acta*, 1997, **42**, 567-577.

ELECTRICAL PROPERTIES OF $As_2 S_3 Ge_8$ - Te THIN FILMS GROWN FROM THE VAPOR PHASE

Marina Ciobanu, Dumitru Tsiulyanu
Technical University of Moldova, Department of Physics, bul. Dacia41, Chisinau 2060,Republic of Moldova
e-mail: ciobmarina@gmail.com

Chalcogenide glassy semiconductors (ChGS) are widely used due to their remarkable physical properties. Unusual properties of these materials originate from peculiarities of their energy spectrum and special chemistry, caused by lone - pair electrons of chalcogen atoms, as well as spatial and compositional disorder. This paper is devoted to study the electrical properties of a complex ChGS from the quaternary system $As_2S_3Ge_8$-Te. Thin films of $As_2S_3Ge_8Te_8$, $As_2S_3Ge_8Te_{13,}$ as well as the functional structures supplied with symmetrical electrodes of different metals, such as In, Au and Pt have been prepared and studied. Thin films were grown from priory synthetized materials, via thermal evaporation in vacuum of 10^{-4} Pa onto Pyrex or sintered Al_2O_3 substrates. The metallic electrodes have been deposited using the same method and similar technological conditions.

The work functions of ChGS in question have been determined and the current-voltage characteristics of the *metal-ChGS-metal* junctions at different polarizations and temperatures were studied. The electrical capacity of such junctions was studied in the frequency range between $5\div10^6$Hz, at different temperatures and different polarities of the applied voltage. The measurements showed a clear dependence of work function on the composition of the chalcogenide material, but for the composition $As_2S_3Ge_8Te_{13}$ it appears to be ≈ 5.03eV. We have found that In, Au, Pt and some Ag pastes form the ohmic contacts with studied thin films. The electrical capacity of the Pt / $As_2S_3Ge_8Te_{13}$ / Pt structure at $< 10^4$ Hz, dependent on the temperature and ChGS chemical composition, increases by more than 4 orders of magnitude with frequency decrease.

Finally, some quantitative parameters of the energetic spectra of $As_2S_3Ge_8$-Te glassy semiconductors were estimated and the energetic diagram of the Pt - $As_2S_3Ge_8Te_{13}$ - Pt functional structure has been designed, using the approach described in [1,2]. It is shown that the forbidden gap monotonically decreases with Te concentration increase as ~ 1.0eV for $As_2S_3Ge_8Te_{13}$ and ~ 0.4eV for $As_2S_3Ge_8Te_{130}$ [3]. Elucidated electrical properties of ChGS in the quaternary system $As_2S_3Ge_8$-Te indicate the possibility of their application to the development of toxic gas sensitive devices for environmental monitoring.

[1] Rhoderick E. Metal-Semiconductor contacts. *Oxford: Clarendon Press*, **1978**.
[2] Tsiulyanu D.I. Formation of the Schottky–Mott barrier on the contact metal-chalcogenide glassy semiconductor. In*: Fiz. Tehn. Poluprovod.*, **1988**, vol. 22, p.1181-1184.
[3] Ciobanu M., Tsiulyanu D. DC conductivity and charge transport in vitreous $As_2S_3Ge_8$–Te films. In: *Chalcogenide Letters*, **2018**, Vol.15, is.1, p.19–24.

GAS FILLED PHOTONIC CRYSTAL RESONATORS: PROPERTIES AND APPLICATION IN SENSING AND METROLOGY

E.Ya Glushko
Institute of Semiconductor Physics,NAS of Ukraine, 41 Nauki prsp. 03028 Kyiv
e-mail: scientist.com eugene.glushko@mail.com

The work is devoted to an approach proposed to determine the universal molar gas constant R with approximately ten significant digits accuracy that is based on extra-accurate volume controlling and high sensitive pressure measurements in the framework of scale echeloning procedure. An essential moment of the method is uniting the results of two connected measurement scales with the relative standard uncertainty near 10^{-5} to obtain a higher precise level. A calibrated stable area of fixed temperature is used in vicinity of the triple point of water. The gas-filled 1D elastic pneumatic photonic crystal is used as an optical indicator of pressure uniting several scales of pressure magnitudes. The pressure gauge includes layered elastic platform, optical fibers and switching valves, all enclosed into a chamber. With this aim, we have investigated the pneumatic photonic crystal bandgap structure and light reflection changes under external pressure.

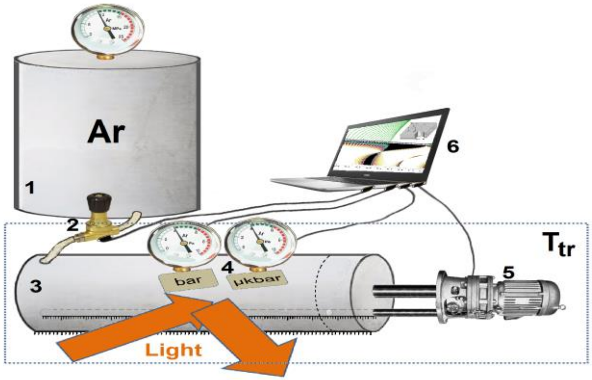


***Fig 1**. Schematically precise pressure indication in the echeloning approach. 1, Inert gas reservoir; 2, controlled lower pressure pump, 3, two-scale volume measurement cylinder calibrated from 0.00005 cm^3 to 4.9999 cm^3 and from 4.9999 cm^3 to 499,999,999.999 cm^3 (1m·0.5 m^2 ; 4, two-scale manometer: 5, plunger position controlling system; 6, main control station. Dotted line, area of stable temperature, triple point of water.*

At the chosen parameters, the two-scale device may cover the pressure interval (0, 10) *bar* with accuracy near *1 nbar*. A self-consistent iteration procedure increasing initial accuracy of parameters and the molar gas constant to the level of volume and pressure accuracy measurements is proposed and tested.

We have also investigated a correlation between spectra of a free pneumatic photonic structure and that deposited on a metal. It was found that for quasi-normal incidence of EMW the presence of metal digs narrow spectral wells in the middle of reflection windows existing for the same free pneumo-photonic crystal. The effects are strongly depended on polarization, number of periods and angle of incidence.

OPTICAL CHARACTERIZATION OF HYBRID PEDOT:PSS/SI HETEROSTRUCTURES BY SPECTROSCOPIC ELLIPSOMETRY

O.S. Kondratenko, S.V. Mamykin, T.S. Lunko, I.B. Mamontova, V.R. Romanyuk
V.E. Lashkaryov Institute of Semiconductor Physics National Academy of Sciences of Ukraine,
41 prospect Nauky, Kyiv 03680, e-mail: kondratenko@isp.kiev.ua

Poly(3,4-ethylenedioxythiophene) blended with poly(4-styrenesulfonic acid) (PEDOT:PSS) is high conducting and high transparent polymer composition having a promising application in the organic electronics and photovoltaics. Spin-coating of aqueous PEDOT:PSS solution with subsequent annealing at ~130°C leads to effective passivation of *n*-Si surface and formation of potential barrier of around 0.7 eV.

The film thickness must be optimized in terms of the formation of antireflective coating of solar cells. Since refractive index at the maximum intensity of the solar spectrum of 550 nm is $n\approx1.5$ the effective film thickness should be near 90 nm. In general, for PEDOT:PSS a gradual growth of conductivity (for about 2 orders of magnitude) is observed with film thickness growth to ~2 μm. Therefore, thin films fabrication with high conductivity is very important for different practical applications.

In this work, the targeted thickness was achieved by applying the multi-step spin-coating procedure, including a washing steps to remove nonconductive PSS phase and other residual fractions from PEDOT:PSS formulation. The thickness and optical parameters (the absorption coefficient *k* and refractive index *n*) of PEDOT:PSS thin films were investigated with spectroscopic ellipsometer SE-2000 (SEMILAB) in the spectral range of 250–2100 nm. By using of the Drude and Cauchy approximation models for $n(\lambda)$, $k(\lambda)$ the spectral fittings of ellipsometric angles (tan Ψ and cos Δ) were performed together with effective layer thickness to minimize the mean-square error between the measured and calculated ellipsometric data.

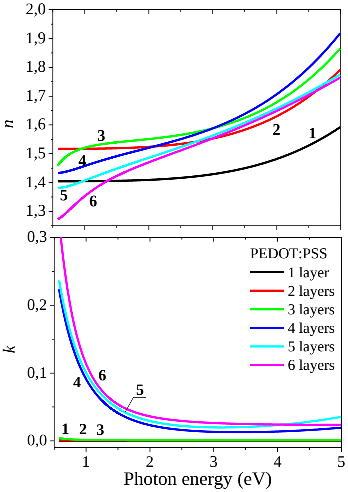


Fig. 1. Spectral dependences of the *n*, *k* of PEDOT:PSS films with a different number of layers deposited on Si substrates.

It was found that the conductivity of the PEDOT:PSS thin film is increased with number of deposited layers, reaching a maximum for the 5-layer film (σ=230 S/cm) and trending to saturation with further steps.

Spectral dependencies of PEDOT:PSS films optical parameters (Fig.1) show that for films of small thickness (1-3 sublayers) spectral behavior of $n(\lambda)$, $k(\lambda)$ is similar to dielectric material, which possibly indicates the large volume fraction of voids in the films. As the number of sublayers increases, in the spectra of $n(\lambda)$ and $k(\lambda)$ a Drude absorption appears at low-energies clearly indicating the improving of electrical contact between the neighboring PEDOT globules.

ELECTRICAL PROPERTIES OF THIN FILMS CdTe DOPED Ca AND Li

Tetiana Mazur[a], Bogdan Dzundza, Volodymyr Prokopiv
[a] *Vasyl Stefanyk Precarpathian National University, Shevchenko Str., 57,*
Ivano-Frankivsk, 76018, Ukraine
e-mail: tetiana.mazur@nung.edu.ua

This paper describes a technique for obtaining thin layers of cadmium telluride p-type conductivity by chemical doping of the surface of CdTe crystals with calcium and lithium. The dependences of the electrical properties of the obtained films on the technological factors of their production are investigated.

As base substrates for obtaining the doped films were used 5×5×2 mm^3 plates, which were cut from a CdTe bulk crystal. The plates were mechanically and chemically polished before doping. Doping was carried out by boiling the substrates in aqueous suspensions of $Ca(NO_3)_2$, $LiNO_3$. The duration of doping process varied from 15 to 60 min. The surface layers change the electronic conductivity to the hole, which is confirmed by a change in the sign of thermo-emf. Measurement of electrical parameters of semiconductor films was carried out on the developed automated device according to the classical method, when a sufficiently high voltage is applied to the sample and the current flowing through the sample is measured.

Since doping only affects the conductivity of the surface layer, the rectangular sample can be considered within the electrical engineering model [1] compared to the impurity distribution over the depth determined from the diffusion equation.

In particular, the parameters of the surface layer and the diffusion coefficient are determined, which are given in Table. 1. The resistivity of the non-alloy material was $6.9\cdot10^5$ Ohm·cm.

Table 1

Parameters doped thin film of CdTe: Ca

The concentration of the solution	%	25	50	75
Specific resistance of film	ρ_g, Ohm·cm	600	900	2400
Concentration Ca in the film	N, sm^{-3}	$1{,}5\cdot10^{20}$	$3{,}0\cdot10^{20}$	$4{,}5\cdot10^{20}$
Diffusion coefficient Ca in CdTe	D, sm^2/s	$3{,}00\cdot10^{-12}$		

Similar studies were performed for cadmium telluride doped with lithium ions.

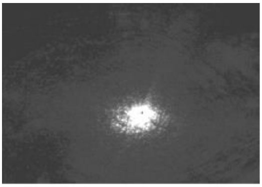
[1] V.V. Prokopiv, O.B. Kostyuk, B.S. Dzundza, T.M. Mazur, L.V. Turovska, O.M. Matkivskyi, M.V. Deychakivskyi. Electrical properties of CdTe<Ca> thin layers, Physics and Chemistry of Solid State, **2019**, 20(4), p. 372-375.

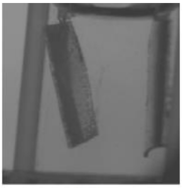
INVESTIGATION OF NANOPARTICLES SOLUTIONS BY OPTICAL METHODS

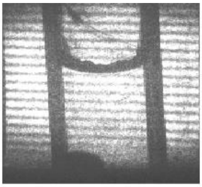
N.A.Davidenko, I.I.Davidenko, N.G.Chuprina, V.V.Kravchenko,
E.V. Mokrinskaya, V.A.Pavlov, S.L.Studzinsky

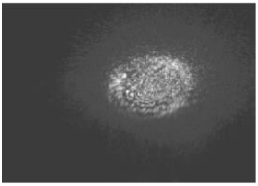
Kiev Taras Shevchenko National University,
Volodymyrs’ka Str., 64, Kiev-01601, Ukraine
E-mail: ndav@univ.kiev.ua

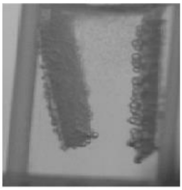
Possibility of application of different optical techniques to reveal presence and to estimate concentration of particles SiO_2 in water solutions is demonstrated in the work. Small sized holographic setup was used for the experimental investigations. Following methods were employed: 1) comparison of light scattering of focused laser beam passed through cuvette with H_2O without nanoparticles SiO_2 and after their introduction into liquid (Fig.1,a and Fig.1,b respectively); 2) observation of electrophoresis process in the cuvette with H_2O without the particles and after their introduction (Fig.2,a and Fig.2,b respectively); 3) holographic technique for observation of the changes of interference stripes for the cuvette with H_2O without the particles and after their introduction (Fig.3,a and Fig.3,b respectively). All 3 methods allow to detect presence of the particles. Increase of their concentration is accompanied by increase of the changes of the optical images. One can suppose that appropriate mathematical apparatus for the images processing will let in future to use considered optical techniques for quick express-analysis of the nanoparticles solutions.

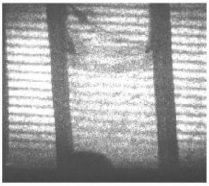

1, a


2, a


3, a


1, b


2, b


3, b

CdTe FILMS AS A MATERIAL FOR SOLAR CELLS: STUDYING THE ELECTRICAL CHARACTERISTICS

Semikina T.V.[a,b], Mamykin S.V.[a], Shmyryeva L.N.[b]
[a] *V. Lashkarev institute of semiconductor physics NAS of Ukraine, Prospect Nauki 41, 03028 Kyiv, Ukraine*
[b]*I. Sikorsky National Technical University of Ukraine "KPI",*
Prospect Peremogy 33, 03056 Kyiv, Ukraine
e-mail: tanyasemikina@gmail.com

The relevance of the preparation and study of polycrystalline films of cadmium telluride (CdTe) is due to the fact that this material is an ideal absorbing material for high-performance and low-cost thin-film polycrystalline solar cells (SC). In most vacuum technological methods (including industrial ones) developed for the deposition of CdTe films, high temperatures of heaters (650–750 °C) and substrates (350–550 °C) are used. Changing technological regimes, one can grow films of both *p*- and *n*-type conductivity. Production of *p*-type films makes it possible to use them in heterojunctions with other materials of A^2B^6 group, which mainly have electronic conductivity type. Despite numerous studies aimed at increasing the conductivity of the films, thin CdTe films used in the manufacture of SCs, as a rule, are undoped.

In the present work, the method of thermal deposition of CdTe polycrystalline films in a quasi-closed space is studied with goal to find the technological regimes that allow to get the CdTe films with charge carriers concentration of order 10^{14}-10^{15} cm^{-3}. By changing the weight of the powder and the diffusion velocity of the moving particles, we changed the partial vapor pressure on the substrate, as well as the molar ratio Te/Cd in the reaction mixture. The carrier concentration was studied in CdTe layers grown on pyroceramic and quartz substrates without the first CdS layer. To determine the type of conductivity, we measured the thermo-electro motion force, which showed that the films have weak *p*-type conductivity. The resistivity of the films was measured using the 4-probe method realized on CHE660E potentiostat. The grown CdTe layers showed the high resistance. The lowest specific resistance value was $\rho = 2.07 \cdot 10^3$ Ω·cm and the highest carrier concentration $p = 3.02 \cdot 10^{11}$ cm^{-3} was observed for a thin film with a thickness of $d = 52$ nm. Technological regimes for the deposition of this layer were low-temperature (480 °C for the evaporator powder CdTe, 400 °C camera, 130 °C substrate) compared with other modes used by us. It could be assumed that the obtained films have a high concentration of defects. It is known the technological regimes determine the dislocation density and the level of microstrains in CdTe polycrystalline films. Thus, we have assumed that the main reason for the high concentration of defects in our films is insufficiently high substrate temperature. The detail discussion regarding the technological parameters effects on obtained electrical properties will be presented.

ADVANCED SPIN-VALVE TYPE NANOSTRUCTURES WITH WEAKLY FERROMAGNETIC AND ANTIFERROMAGNETIC SPACERS

A.I. Tovstolytkin[a], A.F. Kravets[a], D.M. Polishchuk[a,b], Ya.M. Lytvynenko[a], V.Yu. Borynskyi[a] and V. Korenivski[b]
[a]*Institute of Magnetism of the NAS of Ukraine and MES of Ukraine, 36-b Vernadsky Blvd., 03142 Kyiv, Ukraine, e-mail:* atov@imag.kiev.ua
[b]*Nanostructure Physics, Royal Institute of Technology, 10691 Stockholm, Sweden, e-mail: e-mail:* vk@kth.se

Interlayer exchange interactions in spin-valve type magnetic multilayers, such as direct and indirect oscillatory (RKKY) exchange, often dominate the magnetic ordering in the structure. These interactions are essentially fixed and cannot be affected by external parameters post-fabrication. For example, they are proportional to the strength of the magnetization in the ferromagnetic layers and for typical spin-valves vary little for small changes in temperature near room temperature. It would be highly advantageous to be able to affect the strength of the intra-layer and inter-layer exchange interactions in a magnetic stack, as that would result in new types of devices based on magnetic switching via exchange coupling/decoupling of a suitable free layer.

One way to enhance the nanostructure functionalities is to develop spin-valve type multilayers with a temperature-controlled interlayer coupling (the so-called Curie switch or Curie valve), as was suggested in works [1,2]. The Curie switch is a F_1/f/F_2/AF nanostructure where weakly ferromagnetic spacer f is sandwiched between soft magnetic layer F_1 and hard magnetic layer F_2 which is exchange pinned by antiferromagnet AF. In these structures, the coupling between F_1 and F_2 depends on whether temperature T is higher or lower than the Curie temperature of the spacer. As a result, the switching of the net magnetic configuration may be achieved by thermally-controlled driving of the spacer f through its Curie point [2].

The other way to transform the nanostructure functionalities is to use antiferromagnet-mediated interactions in layered nanostructures “hard ferromagnet/ antiferromagnet/ soft ferromagnet”. For these nanostructures, unexpectedly peculiar behavior has been revealed in the vicinity of the antiferromagnet ordering temperature.

In this work, the results obtained on both kinds of layered nanostructures, with weakly ferromagnetic and antiferromagnetic spacers, will be presented and discussed.

The new data are believed to contribute to the optimization spin-valve-based magnetic nanostructures and pave the way for the development of novel elements and devices of nanoelectronics and spintronics.

[1] A.F. Kravets *et al*. *Phys. Rev. B*, **2012**, v. **86**, 214413 (1-7).
[2] D.M. Polishchuk *et al*., *Phys. Rev. B*., **2018**, v. **98**, 144401 (1–8).

EFFECT OF LOW MOLECULAR WEIGHT ARENES ADDITIVES ON THE INTERPHASE LAYER STRUCTURE OF SAN-PS SYSTEMS AND DIELECTRIC BEHAVIOR OF SUCH COMPOSITIONS

Anoshenko M.[a], Bazylyuk T.[a], Iukhymenko N.[a], Budzinska V.[b]
[a] *Faculty of Chemistry, Macromolecular Chemistry Department, Taras Shevchenko National University of Kyiv, Kyiv, 01033, 60 Volodymyrska Street, Ukraine.*
e-mail: yukhimenko.n@gmail.com
[b] *Institute of Macromolecular Chemistry of National Academy of Sciences of Ukraine, 48 Kharkivs'ke shose, Kyiv 02160, Ukraine, e-mail: budzinska@meta.ua*

The aim of this work was to study the low molecular weight arenes (LMWA) influence on the dielectric behavior of binary system with limited compatibility between components based on styrene-acrylonitrile copolymers (SAN) – polystyrene (PS). It could be expected that the LMWA will enhance the interphase layer (IPL) due to the π-π electron conjugation of the phenyl groups of components and, respectively, intermolecular interaction (IMI) in the IPL.

The industrial thermoplastic polymers SAN of azeotropic composition and suspension PS were used in the work.

The benzene, toluene, styrene, benzonitrile (BN) were used as low molecular weight components. LMWA were incorporated into a polymer matrix by sorption of the corresponding liquid under saturated vapor (desiccator method). The amount of low molecular weight substances incorporated into polymers were ~ 0.5% wt. % relative to the polymer matrix.

The following dielectric parameters, such as the tangent of the dielectric loss angle (tg δ) and dielectric permittivity (ε'), were estimated. Conclusions about the basic mechanisms of intermolecular interaction changing in the IPL were made based on the FTIR spectroscopy data. IR spectroscopic investigations were carried out in the range 400-4000 cm^{-1}.

It was established that benzene interacts selectively with SAN and PS, blocking the polymer-polymer interaction in the IPL.

The IPL structure rearrangement in the presence of toluene, as well as the growth of the stabilization of lyophilic fluctuating network which forms the IPL was detected.

Styrene can be used as a compatibilizer of investigated polymer-polymer system.

Benzonitrile causes a weakening of the intermolecular interaction in the IPL due to the selectivity (similarly to benzene), as well as the dipole-dipole interaction of the nitrile groups of copolymer and benzonitrile. The complex IPLs structure is formed by competing (lyophilic and lyophobic) fluctuation networks. It was concluded that the rigid lyophobic network formation possibility, as well as the connected with this process mixtures heterogeneity сумішей is controlled, in general, by the SAN content in the compositions.

GROWTH, CRYSTAL STRUCTURE AND OPTICAL PROPERTIES OF Al-DOPED ZnO THIN FILMS

A. Kashuba[a], H. Ilchuk[a], R. Petrus[a], B. Andriyevsky[b], O. Bovgyra[c], I. Semkiv[a],
M. Kovalenko[c], V. Dzikovskyi[c]
[a] *Department of General Physics, Lviv Polytechnic National University, 12, S. Bandera Str., Lviv-79013, Ukraine*
[b] *Faculty of Electronics and Computer Sciences, Koszalin University of Technology, 2, Śniadeckich str., PL-75-453, Koszalin, Poland*
[c] *Faculty of Physics, Ivan Franko National University of Lviv, 8a, Kyrylo and Mefodiy St., Lviv, UA–79005, Ukraine*
e-mail: AndriyKashuba07@gmail.com

Zinc oxide (ZnO) is an important material in many optoelectronic devices with wide applications such as varistors, biosensors, gas sensors, transparent electrodes, etc. ZnO is normally introduced and doped with group III elements such as B, Ga, In or Al in order to improve and develop optical transmittance and optical energy band gap of ZnO thin films by modifying its electrical, optical and other properties. Al-doping concentration played a major role on the enhancement of transparency and the shift of optical band gap of ZnO thin films.

Al-doped ZnO (ZnO:Al) thin films prepared by high-frequency magnetron sputtering method. The glass substrates were ~14 mm in diameter were used for deposition ZnO:Al thin films. Before the films deposition, the substrate surface was cleaned by boiling in a high purity CCl_4 solution during 0.5 h.

The phase analysis and crystal structure refinement was examined with using X-ray diffraction data. The mean grain size was determined using the Scherrer formula. The strain and the dislocation density are also calculated.

Chemical composition of the films was examined using energy dispersive spectroscopy (EDS). The surface morphology of the obtained ZnO:Al films was studied using a JSM 6700F scanning electron microscope.

The spectral dependence of the optical transmittance (Shimadzu UV-3600) of the obtained samples in the visible and near infrared regions is studied at room temperature [1]. The optical constants and the band gap of the films under study have been determined. Optical properties (refractive index $n(\lambda)$, absorption coefficient $\alpha(\lambda)$, extinction coefficient $k(\lambda)$, dielectric functions $\varepsilon(\lambda)$ and optical conductivity $\sigma(\lambda)$) of thin films and thickness d can be determined from the transmission spectrum.

[1] R.Yu. Petrus, H.A. Ilchuk, A.I. Kashuba, I. Semkiv, E. Zmiiovska, *Optics and Spectroscopy.*, **2019**, 126(3), 220.

ELECTRICAL PROPERTIES OF ZnO THIN FILMS DEPOSITED BY RF-MAGNETRON SPUTTERING

Semikina T.V.[1,2], Vasin A.V. [1,2], Rusavsky A.V. [1,2], Mamykin S.V.[1], Nazarov A.N. [1,2]
[1]V. Lashkarev institute of semiconductor physics NAS of Ukraine, Prospect Nauki 41, 03028 Kyiv, Ukraine
[2]National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Prospect Peremogy 33, 03056 Kyiv, Ukraine
e-mail: tanyasemikina@gmail.com

ZnO is an intensively studied wide band gap semiconductor material for applications in electronics and photovoltaics, generally for use as a transparent conductive material. There are numerous technological methods used to deposit ZnO: pulse laser deposition (PLD), radio-frequency and dc -magnetron sputtering, reactive sputtering, metal-organic chemical vapor deposition, sol-gel method, the atomic layer deposition method (ALD). This work is devoted to deposition of ZnO thin films by RF magnetron sputtering and studying of their structural and electrical properties. The novelty of this work is based on usage of methane in reaction chamber that resulted in high conductivity of obtained films without doping by typical dopants like as Al, N, Ga.

Zinc oxide thin films were deposited on silicon and optical glass. The compacted ZnO powder (99.9% purity, grain size about 5 μm) was used as a sputtering target. The sputtering chamber was evacuated to a base pressure of $3\cdot10^{-4}$ Pa followed by introducing working gas that was pure argon gas (9 sccm), argon (9 sccm)/oxygen(2 sccm) or argon(9 sccm) /methane(2 sccm) keeping working pressure at about 10^{-1} Pa. During the sputtering process, substrate temperature was about 200 °C, target-to-substrates distance was 70 mm, and RF discharge power was 190 W.

The electrical measurements were carried out by 4-probe method realized on CHE660E potentiostat. As the results we have got the values of sheet resistance R_{sh}, specific resistance ρ_{sp} and concentration of carriers n. The highest resistances ($R_{sh} = 5{,}21\cdot10^{12}$ Ohm/SQ, $\rho_{sp} = 2{,}85\cdot10^{6}$ Ohm·m for glass substrate and $R_{sh} = 2{,}2\cdot10^{10}$ Ohm/SQ, $\rho_{sp} = 1{,}17\cdot10^{4}$ Ohm·m for silicon wafer) were obtained for films deposited in gas mixture of $Ar+O_2$, and the lowest values ($R_{sh} = 3{,}71\cdot10^{3}$ Ohm/SQ, $\rho_{sp} = 2{,}62\cdot10^{-3}$ Ohm·m for glass substrate and $R_{sh} = 110$ Ohm/SQ, $\rho_{sp} = 6{,}45\cdot10^{-5}$ Ohm·m for silicon substrates) were obtained in $Ar+CH_4$ environment. Similarity, the highest concentration of charge carriers $n = 1{,}4\cdot10^{18}$ cm^{-3} for glass substrtates and $n = 5{,}7\cdot10^{19}$ cm^{-3} for silicon substrates were obtained for ZnO films deposited in $Ar+CH_4$. The lowest values $n = 1{,}29\cdot10^{9}$ cm^{-3} for glass and $n = 3{,}14\cdot10^{11}$ cm^{-3} for silicon substrate were observed for case of $Ar+O_2$. The effect of substrate nature, gas content on structural and electrical properties will be discussed. The model of defects formation will be suggested.

THIN SOLID FILMS OF PHOSPHORYLATED CALIX[4]ARENES: STRUCTURE AND SENSORY PROPERTIES

Z.I. Kazantseva [a], I.A.Koshets[a], V.I.Kalchenko[b]

[a] *Institute of Semiconductor Physics, National Academy of Sciences of Ukraine, pr.Nauki 45, Kiev-39, Ukraine*

[b] *Institute of Organic Chemistry, National Academy of Sciences of Ukraine, Murmanskaya st.5, Kiev-94, Ukraine*

e-mail: kazants@isp.kiev.ua

Nowadays a great attention is paid to creation and development of miniaturized, low-cost, smart chemical sensing systems based on various physical and chemical principles, which provide accurate and reliable real-time control of ambient medium. One of the most important problems under creation of such systems (known as “Electronic noses”) for pattern recognition of smells is the choice of appropriable sensitive materials for coating of sensor. Requirements that should be met with these layers are quite versatile and even contradictions. From the one hand sensor should provide good and quick response to the presence of analyzed molecules in surrounding air, from the other hand sensor must have sensitivity to the interfering molecules as less as possible. As well, sensor should be easily cleaned. From this point different types of functionalizated calixarenes are very promising materials and many researchers focus their attention on investigation of selective and sensitive properties of calixarene films.

This work reports on the results of investigation of quarts crystal microbalance (QCM) sensors coated with novel phosphorylated calixarenes (CA) to wide range of volatile organic molecules. The influence of introduction of various functional groups into calixarene molecule macrocycle to sensitivity towards different organic molecules has been analyzed. Sensors coated with phosphorous-containing calixarenes showed a high sensitivity and an excellent selectivity towards volatile organic compounds (aromatics, chlororganics, ketones and aliphatic alcohols). Sensor response was found to be depended on chemical structure of calixarenes under study, particularly, on the substituting group of molecule. Good sensor response has been obtained for all CA compounds. Concentration dependencies and sensitivity thresholds of sensors have been obtained. Detection limit of several analytes was less than 10 ppm.

Films of the phosphorylated calixarenes demonstrated fast and reversible adsorption to wide range of analyte except the situation when stable complex “host-guest” was formed. The phosphorylated calix[4]arenes were synthesized in the Institute of Organic Chemistry in Kiev. The chloroform solutions of calixarenes were used for deposition onto quartz crystals by different technologies.

NANOSTRUCTURED CuI THIN FILMS ON BIODEGRADABLE NANOCELLULOSE FLEXIBLE SUBSTRATES FOR UV-SHIELDING APPLICATIONS

N.P. Klochko [a], V.A. Barbash [b], K.S. Klepikova [a], V.R. Kopach [a], O.V. Yashchenko [b],
D.O. Zhadan [a], S.I. Petrushenko [c], S.V. Dukarov [c], V.M. Sukhov [c], A.L. Khrypunova [a]

[a] National Technical University “Kharkiv Polytechnic Institute”, 2, Kirpichov st., 61002 Kharkiv, Ukraine, e-mail: klochko.np16@gmail.com
[b] National Technical University of Ukraine “Igor Sikorsky Kyiv Polytechnic Institute”, 37, Prospect Peremohy, 03056 Kyiv, Ukraine
[c] Kharkiv National University named after V. N. Karazin, 4, Svobody Square, 61022, Kharkiv, Ukraine

Ultraviolet radiation (UV) triggers the formation of free radicals, and as a result, the long-term exposure of human skin to UV radiation may cause health issues, such as aging, DNA damage, skin reddening, and even skin cancer. UV light has also degradation effects on various materials, such as polymers, dyes, pigments and semiconductor devices. This explains an interest in the creation of lightweight and flexible biodegradable (without accumulating debris) shields with variable shapes, which are capable of providing protection from the solar UV. In this work, we study a suitability for protection against terrestrial ultraviolet part of the solar spectrum of cuprous iodide (CuI) films obtained via cheap, affordable, and suitable for mass production aqueous method Successive Ionic Layer Adsorption and Reaction (SILAR). As lightweight low-cost flexible substrate for these UV-shields we propose a new eco-friendly plant-derived nanocellulose (NC) film, which should become a biodegradable alternative to common petroleum-based polymer tapes. As a raw material for production of NC substrates, we use fast-growing perennial herb Miscanthus x giganteus. To manufacture of nanocellulose films, we use an environmentally friendly method of organosolv delignification of plant raw materials carried out at a low temperature and in a relatively short time.

The morphology of NC and CuI observed by scanning electron microscopy (SEM) and atomic force microscopy (AFM). Chemical compositions of the films investigated by X-ray fluorescence (XRF) microanalysis and Fourier transform infrared spectrophotometer (FTIR). To research crystal structure we use X-ray diffraction (XRD) method. The UV-protection ability of the nanostructured CuI thin films, on NC substrates have been evaluated on the base of their optical properties in accordance with an international standard ISO 2443:2012(E) “Determination of sunscreen UVA photoprotection in vitro”.

According to the research, nanostructured CuI thin films made by the low-cost and suitable for large-scale production SILAR method on the thin flexible biodegradable nanocellulose substrates have been proposed as a new material for UV-shielding applications. In accordance with an international standard ISO 2443:2012(E), UV-protection ability of the samples consisting of the NC substrates and CuI films deposited on them by the SILAR method fits the category “excellent” (50^+).

CARBON SCREEN PRINTED ELECTRODES MODIFIED WITH COMPOSITE FILMS BASED ON SILICA FOR H_2O_2 DETERMINATION

Anastasiia Kornii, Anna Borets, Vladyslav V. Lisnyak, Oksana Tananaiko
Department of analytical chemistry, Taras Shevchenko National University of Kyiv, 64, Volodymyrska str., Kyiv 01601, Ukraine
e-mail: anastasiiakovalyk@ukr.net

Silica-based materials have attractive features due to the versatility of sol-gel processing for the development of electrochemical sensors. Manganese (II) oxide and copper (II) oxide particles possess a catalytic activity toward hydrogen peroxide. Graphen oxide (GO) is promising modificator thanks to its high effective surface area and electrochemical activity.

The objective of this work is the development of sensitive and selective sensor elements for the hydrogen peroxide determination. For this purpose, the sreeen printed carbon electrodes (SPCE) were modified with composite films $MnO_2/GO/SiO_2$ and $CuO/GO/SiO_2$ by electroassisted deposition (EAD) method.

MnO_2 particles were obtained by electrodeposition from aqueous solution of Mn(II) onto SPCE surface. The obtained SPCE/MnO_2 electrode was cowered with a silica film which contained GO particles. The SPCE/MnO_2/GO/SiO_2 was obtained. Copper (II) oxide particles were obtained by hydrolysis of Cu(II) solution. then SPCE electrode was modified with composite silica film contained CuO particles and GO.

The morphology of the MnO_2 and CuO particles was observed by scanning electron microscopy. The MnO_2 particles were uniformly distributed onto the electrode surface, had a round shape and were 190-250 nm in diameter. The CuO were roughly about 100±50 nm in diameter. It was also investigated CuO morphology in SiO_2 film. Silica film was uniformly fixed on the surface of the electrode and CuO particles were evenly distributed in it. Additional aggregation of particles on the surface in the SiO_2 film was not observed.

The electrochemical characteristics of the modified electrodes were investigated by cyclic voltammetry. The presence of MnO_2 on the surface of modified electrode was indicated by the appearance of clear oxidation peak of Mn(IV)/Mn(III, II) at E=0,7 V in the buffer solution in contrast to unmodified electrode. The presense of CuO particles onto SPCE surface was indicated by the appearance of oxidation-reduction peaks $E_{Ox} = -0.16$ V and $E_{Red} = -0.5$ V of Cu(II)/Cu(I). The oxidation- reduction current increases in the presence of GO particles on the surfcae of the electrodes. Optimization of the parameters of modification of SPCE such as the amount of MnO_2 and CuO, pH value, were studied. Under the optimum conditions, the calibration curve for H_2O_2 determination using SPCE/MnO_2/GO/SiO_2 electrode was linear in the range of 0,005-0,5 mM with a detection limit of 0,003 mM (S/N = 3). The linear range for H2O2 calibration cureve at SPCE/CuO/GO/SiO_2 electrode was 0,05-0,3 mM with a detection limit of 0,03M (S/N = 3).

The developed SPCE electrode modified with CuO/GO/SiO_2 and MnO_2/GO/SiO_2 are perspective sensitive elements of voltammetric sensors for H_2O_2 determination.

ULTRA-THIN SILICON TEXTURING FOR FLEXIBLE PHOTOVOLTAICS

Viktoriia Koval, Mykhailo Dusheyko, Valerii Barbash
National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute",
37 Prosp.Peremohy, Kyiv,03056, Ukraine
e-mail: v.m.koval@kpi.ua

For highly efficient solar cells a diffusion length of charge carriers has to exceed in several times material thickness. Nowadays, it is observed a shift in wafer production towards thinner substrates than the traditional thickness of 400-500 μm. The optimum values of substrate thickness for ultra-thin solar cells lay in a range of 50 – 100 μm [1]. Besides, ultra-thin silicon is characterized with enough flexibility and can be used to develop of flexible thin-film solar cells. But during standard chemical texturing operation in PV-production, a layer of 10 to 15 μm is removed from silicon surface that is not acceptable for ultra-thin substrates [2]. The texture size of ultra-thin substrates has not to exceed 1-2 μm, so submicron texturing process is need to develop.

To obtain ultra-thin silicon substrates the potassium hydroxide solution was used. Silicon substrates were thinned up to 50 - 100 μm and then subjected to the texturing process. Commonly-used alkali solutions were complemented with isopropanol and ethylene glycol as surfactants to achieve the submicron texturing. In order to obtain solar cells, silicon thin films were deposited on texturized ultra-thin silicon substrates using ion-beam sputtering technology. PV front contacts were produced as multilayer structure of Ti/Mo/Ag and PV rear contact was deposited as continuous film of Al using RF magnetron sputtering.

In this work the influence of ethylene glycol content in texturing etchant on silicon surface morphology and optical reflectivity was investigated. It was shown that the addition of surfactants (0,5 – 5 ml) led to obtain of low-height pyramids on textured surface (0.4 – 1.6 μm). Minimum value of reflectance (< 10%) is observed for just submicron textured silicon surface. Also, it has been established that reducing of wafer thickness from 500 to 90 μm (without any texturing) causes the increase in short-circuit current from 220 to 250 μA. Application of submicron texturing resulted in further increase in short-circuit current up to 380 μA. It should be noted that ultra-thin silicon, textured in standard solution, provided significant deterioration of short-circuit current from 280 to190 μA, that can be due to breaking of thin silicon films on this developed surface. So, ultra-thin silicon wafers with submicron texturing were obtained and used to design of flexible thin-film silicon solar cells.

[1] Kowalczewski P. et al "Towards the efficiency limits of silicon solar cells: How thin is too thin?", *Solar Energy Materials & Solar Cells*, **2015**, Vol. 143, pp. 260-268.

[2] Dewan R. et.al. "Light trapping in thin-film silicon solar cells with submicron surface texture", *Optical Society of America*, **2009,** Vol. 17, pp. 1-10.

STRUCTURE OF DIAMONDOID THIOL MONOLAYERS ON GOLD: AN STM STUDY

Ya.Yu. Lopatina[1,2], T.S. Zhuk[2], A.A. Fokin[2], A.A. Marchenko[1]
[1] *Department of Physical Electronics, Institute of Physics of NAS of Ukraine,*
Nauky ave, 46, Kyiv-03039, Ukraine
[2] *Department of Organic Chemistry, National Technical University of Ukraine "KPI",*
Peremohy ave, 37, Kyiv-03056, Ukraine
e-mail: yaroslava.lopatina@gmail.com

Diamondoids are cage molecules, belongs to homological series with a structural unit of an elementary cell of diamond crystal ($C_{4n+6}H_{4n+12}$). Due to electronic and optical properties these molecules are of interest for molecular electronics [1,2], as building block for more complex systems etc. For technological application, diamondoids are functionalized by surface-reactive units, in particular SH-groups. However, previous studies of lower thiolated diamondoids – adamantane (n=1) and diamantane (n=2) – have revealed that structure and stability of monolayers is determined by the position of the SH-group on the cage of the molecule [3,4].

Considering both fundamental and practical interest, we aim to continue investigation of thiolated diamondoid thiol and report the results of comparative STM study of triamantane-thiol derivatives (Fig.1) monolayers, chemisorbed on Au(111) surface.

2SH **3SH** **9SH**

Fig.1. Structure of triamantane-thiols.

[1] Monochromatic Electron Photoemission from Diamondoid Monolayers, *Science*, **2007**, 316, 1460-1462.

[2] Monochromatic Photocathodes From Graphene-Stabilized Diamondoids, *Nano Lett.*, **2018**, 18(2), 1099-1103.

[3] Near-Edge X-ray Absorption Fine Structure Spectroscopy of Diamondoid Thiol Monolayers on Gold, *J.Am.Chem.Soc.*, **2008**, 130, 10536-10544.

[4] Structure and Dynamics in Monolayers of Thiolated Diamantane Derivatives, *J.Phys.Chem.C*, **2019**, 123(45), 27477-27482.

SUPERHYDROPHOBIC TEXTILES WITH FIBERS COATED BY NANOSCTRUCTURED INDIUM-DOPED ZINC OXIDE LAYERS

N.P. Klochko [a], I.V. Khrypunova [a], K.S. Klepikova [a], V.R. Kopach [a],
D.O. Zhadan [a], S.I. Petrushenko [b], S.V. Dukarov [b], V.M. Lyubov [a], M.V. Kirichenko [a]
[a] *National Technical University “Kharkiv Polytechnic Institute”, 2, Kirpichov st., 61002 Kharkiv, Ukraine e-mail: klochko.np16@gmail.com*
[b] *Kharkiv National University named after V. N. Karazin, 4, Svobody Square, 61022, Kharkiv, Ukraine*

The use of nanostructured doped and pristine zinc oxide (ZnO) thin layers for the functionalization of textile substrates is growing rapidly, since ZnO can provide unique multifunctional properties, such as photocatalytic self-cleaning, antimicrobial activity, protection against ultraviolet radiation, flame retardancy, electrical conductivity, thermal insulation, and superhydrophobisity. The superhydrophobic surfaces or materials are those, which have an excellent water repellent ability called “lotus effect”. An advanced “green” lifestyle asks for textiles that can be self-cleaning, for instance, mimicking the superhydrophobic lotus leaf in nature, in order to save on the use of detergent and labor. So, there are strong demands for simple, low-cost and massive product techniques for the homogeneous and controlled loading of ZnO nanostructures on the commercial fabrics.

In this study by means of the low-temperature cheap and scalable method Successive Ionic Layer Adsorption and Reaction (SILAR) for a deposition of nanostructured indium-doped zinc oxide (ZnO:In) thin films we obtained comfortable to wear, breathable, nontoxic, light-weight, flexible and air-permeable textile on the base of cotton (Ct) and polyester (Pe) fabrics without any addition impregnation layers for a hydrophobic modification. To ensure superhydrophobicity, the ZnO/Ct and ZnO/Pe tissues were subjected to a post-growth vacuum annealing.

The morphology of Ct and Pe fabrics, and of the ZnO:In/Ct and ZnO:In/Pe textiles observed by scanning electron microscopy (SEM). Their chemical compositions investigated by X-ray fluorescence (XRF) microanalysis. To research crystal structure we use X-ray diffraction (XRD) method. Optical properties of ZnO:In in the ZnO:In/Ct and ZnO:In/Pe textiles investigated using UV-Vis-NIR spectrophotometer. For a research of surface hydrophilicity/hydrophobicity conversion were used conventional sessile drop method and tilt angle measurements. SEM images and XRF data demonstrate an uniform coating of external and internal fibers of tissues by ZnO:In films in both ZnO:In/Ct and ZnO:In/Pe textiles. Analysis of XRD patterns of the ZnO:In/Ct and ZnO:In/Pe textiles has revealed that all ZnO:In films are single-phased, nano-grained and have polycrystalline wurtzite hexagonal ZnO structure (JCPDS #36-1451). The obtained from the Kubelka-Munk function for the SILAR deposited ZnO:In films in the ZnO:In/Ct and ZnO:In/Pe tissues optical band gap values for direct transitions are close to the ones characteristic for bulk zinc oxide.

Analysis of crystal structure, morphology, chemical composition and optical properties together with data about contact angles of the water drops on the ZnO:In/Ct and ZnO:In/Pe surfaces allowed us to select SILAR modes and vacuum annealing conditions to obtain the superhydrophobic textiles with fibers coated by ZnO:In thin films without additive impregnation layers.

DESIGN AND CHARACTERIZATION OF FUSED IMINOPYRIDINE POLYMER-BASED FLUORESCENT PROBES

Makeiev A.M., Milokhov D.S.,
Keda T.Ie., Khilya O.V., Volovenko Yu.M.
Taras Shevchenko National University of Kyiv, 01601, Kyiv, Volodymyrska St., 64/13;
e-mail: makeev_a@ukr.net

Due to the peculiarities of the fluorescent method, fluorescent probes and sensors are widely used for various tasks of analytical chemistry, especially in clinical diagnostic and biological studies, environmental monitoring. Polymer-based films with fluorophores are advantageous over liquid probes, providing the express analysis, automation and simple equipment design.

It has been shown previously that fused iminopyridine derivatives fluorescence characterized by satisfactory quantum yields in various solvents. Acidity changing affects the fluorescent properties of these compounds, that leads to an increase or quenching the luminescence intensity of fluorophores in solution. This effect was used for developing liquid-phase acidimetric sensor systems.

In this work it was shown the design and synthetic approach of hydrophilic polymer films based on 2-hydroxyethyl methacrylate copolymers modified with pH-sensitive fused iminopyridine derivatives[1]. The developed technique of express one-step films synthesis was tested on new fluorophore. Fluorescent properties of the film obtained were studied. The influence of aqueous solutions acidity on analytical response of films, the ability to regeneration, selectivity of the obtaining materials and the possibility of reuse were shown. Comparative characterization of dyes based on two and three fused iminopyridines was submitted. The data obtained indicate the possibility of using developed systems for fluorescence sensing of aqueous medium acidity.

1. A method of fluorescence determination of pH of gastric juice // Patent of Ukraine №12054, 10.12.2019, bul. №23

DETERMINATION OF Pb(II) CONCENTRATION IN AQUEOUS MEDIUM ON NANOCRYSTALLINE TiO_2/Y THIN-FILM ELECTRODE

I. Medyk[a], V. Vorobets[b], G. Kolbasov[b], A. Garashchenko[a], S. Oblovatna[b], S. Karpenko[b], N. Antonyuk[a]

[a]*National University of „Kyiv-Mohyla Academy". Skovoroda str., 2, Kyiv-04070, Ukraine*
[b]*Vernadsky Institute of General and Inorganic Chemistry of the NAS of Ukraine.*
Acad. Palladin Str., 32/34, Kyiv-03142, Ukraine
e-mail: vorobetsvs@i.ua

We present study results of possibility to use electrodes based on nanocrystalline Y-doped titanium oxide thin films to determine the concentration of Pb^{2+} ions by anodic stripping voltammetry method. This method consists in preliminary electroconcentrating of Pb^{2+} ions in cathodic potential range and subsequent electrodissolution of electrodeposition products at anode potential scan.

Thin films based on nanocrystalline titanium oxide modified by Y were produced by sol-gel method on Ti substrate from solutions containing titanium isopropoxide, ethanol, acetic acid, yttrium nitrate and surfactant (Triton X-100); after which the electrodes were annealed in air at 500°C. The prepared samples were characterized by using X-ray diffraction and ultraviolet-visible photocurrent spectra. The average size of nanoparticles calculated from the Scherrer equation was 7- 11 nm. The XRD results indicated that TiO_2/Y electrodes calcined at 500°C consisted of anatase as the unique phase. The photocurrent spectra of the TiO_2/Y electrodes ($0 \le$ Y concentration ≤ 5 mol%) showed a stronger current in the UV range and doping with yttrium shifts the photocurrent spectra to the long-wave region of the spectrum.

Determination of Pb(II) was done using background solutions based on 0.35 M formic acid, 0.1 M hydrochloric acid and acetate buffer (pH = 5.0) using standard addition method with potential scanning speed of 20–50 $mV \bullet s^{-1}$. The solution was stirred during the preliminary electroconcentrating at potential of –(1200–1600) mV (vs silver-chloride reference electrode) for 60– 180 seconds and then the potential was scanned from -1600 mV to + 200 mV. It is shown that TiO_2–Y electrodes can be used as indicator electrodes for determination of Pb(II) by anodic stripping voltammetry method. Optimum conditions of Pb(II) determination are: background solution is acetate buffer (pH = 5.0), electroconcentrating potential -1,4 V; time of electrolysis 120 s, scanning speed of potential 50 $mV.s^{-1}$. By means of this method it is possible to determine the concentration of Pb(II) within (0,02-5,30) $mg.l^{-1}$.

PECULIARITIES OF $CuInSe_2$ LAYERS FABRICATION

V. Nicorici, P. Chetrus
Moldova State University, str. Alexei Mateevici, 60, Chisinau MD-2009, Moldova
e-mail: vnicorici@yahoo.com

The ternary $CuInSe_2$ compounds (CIS) with the chalcopyrite crystal lattice are promising materials from the point of view of creating effective photo-converters based on them. However, there are difficulties in obtaining CIS layers with the necessary predefined parameters, which will make it possible to obtain solar cells with efficiency up to 20% [1]. Upon heating, the CIS compound dissociates into copper and indium selenides, which at a deposition temperature have different saturated vapor pressure P_s. This leads to a change in the composition of the obtained layers in comparison to the composition of the source.

The influence of the obtained method on the crystalline structure and electrical was studied for the determination of the optimal technological conditions. CIS thin layers were obtained by two methods: "flash" evaporation method and the so-called "shell method". CdS crystals or mica were used as a substrate.

By using the first method [2] the semiconductor material, which needs to be evaporated, is injected into the system in the form of very small granules, and the temperature of the evaporator, on which these granules fall, is set in such a way that the least volatile component evaporates. Due to the reduced thermal capacity of each granule, it evaporates quickly and almost completely. As a result layers have approximately the same composition as the source material. The layer growth rate was 0,2…0,5 μm/min and the layers thickness – 1…5μm with the dimension of the grains – 0,2 – 0,4 μm in diameter.

In the case of the "shell" method the cell - evaporator has the shape of a cylinder coiled into a spiral and closed from the sides, with the single adjustable opening through which evaporation occurs. Thus, the shape of the evaporating cell repeats the shape of the shell. The cross-sectional area of the cylinder is much smaller than its surface; therefore, at a constant temperature of the evaporator, the molar - kinetic characteristics of the vapor flow are independent of the mass of the material and the deposition time. The layer growth rate was 0,4 …0,7 μm/min, the layers thickness reached ~15μm and the dimension of the grains was 0,5 – 0,7 μm. Thus, layers with a polycrystalline structure were obtained in both methods.

All layers conductivity was of p-type. Electrical conductivity and hole concentration temperature dependences were studied in the temperature range of 80 - 400K. $CuInSe_2$ layers fabricated by "flash" method had the hole concentration of $p \approx 4 \cdot 10^{19} cm^{-3}$, and the layers fabricated by "shell method" had the hole concentration of $p \approx 10^{17} cm^{-3}$ at T=300K.

1. Г. С. Хрипунов и др. *ФТП*, **2014**, N12, c.1671-1675.
2. V.Nicorici, P. Chetrus. *PLUMEE*, **2017**, N 1, p.7-8. (ISSN 2343-9092).

THE INFLUENCE OF THE LIGAND NATURE ON THE ELECTROCHEMICAL PARAMETERS OF THE TIN FILMS AS ANODE MATERIALS FOR LITHIUM ION BATTERIES

V.S. Kublanovsky [1]*, N.I. Globa [2]**, V.M. Nikitenko [1], E.A. Babenkov [1],
Yu.V. Shmatok [2]
*[1]Vernadskii Institute of General & Inorganic Chemistry of National Academy of Sciences of Ukraine, Palladina ave, 32/34, Kyiv, 03142, Ukraine;*e-mail: kublan@ukr.net*
*[2]Joint Department of Electrochemical Energy Systems of NAS of Ukraine, Vernadskogo blvd, 38a, Kyiv, 03680, Ukraine;**e-mail: gnl-n@ukr.net*

The development of new anode materials that provide high values of specific capacitance and discharge current density is an urgent task. A possible alternative to carbon materials is the use of thin tin electrolytic films, tin based composites and tin alloys with nickel, copper, cobalt, bismuth, antimony in lithium-ion batteries (LIB). Tin and its alloys are promising anode materials for LIB, since tin has low discharge potential and $Li_{22}Sn_5$ alloy has high theoretical specific capacity ($994\ mA \cdot h \cdot g^{-1}$).

The scientifically substantiated selection of ligands for complex, including polyligand, electrolytes makes it possible to control the inhibition of the electrode process and, consequently, the structure and functional properties of the obtained coatings with metals and alloys.

We have developed technological processes of electrolytic deposition of functional tin films from tartrate (KNatart), citrate (Na_3cit), citrate-trilonate (Na_3cit / Na_2H_2edta) and pyrophosphate ($K_4P_2O_7$) electrolytes. The influence of the ligand nature, current density, and mass of tin coating on the electrochemical characteristics of tin films during the LIB cyclization is investigated.

Depending on the nature of the ligand, the current magnitudes of the peaks of intercalation-deintercalation of lithium into tin films decrease in the sequence: $tart^{2-} < cit^{3-} < cit^{3-}/edta^{4-} < P_2O_7^{4-}$ ions. The nature of the ligand determines the composition of electrochemically active complexes (EAC), the mechanism of the process, the morphology and electrochemical characteristics of tin films, in particular the magnitude of the specific discharge capacity and corrosion resistance as the anode materials of LIB. The effect observed can be explained by the change in the structure of tin films obtained from complex electrolytes, in accordance with the increase in the stability of the tin (II) complexes formed in this series. This in turn determines the size of the tin particles and the density of their packing.

The most stable electrochemical characteristics (specific capacitance, stability, and ability to reverse cycling in LIB) are inherent in tin films obtained from pyrophosphate (650-700 $mA \cdot h \cdot g^{-1}$) and citrate (500-530 $mA \cdot h \cdot g^{-1}$) electrolytes based on tin chloride (II). Higher specific characteristics of these tin films during the introduction and extraction of lithium are caused by the mechanism of their production. The process of deposition of tin (II) from the pyrophosphate electrolyte depending on the pH of the solution is limited by the preliminary chemical reaction of dissociation of protonated $[Sn(HP_2O_7)(P_2O_7)]^{5-}$ (pH 4.5) or non-protonated $[Sn(P_2O_7)_2]^{6-}$ (pH 7.2) complexes. This allows to control the morphology, structure and functional properties of the obtained tin films.

GROWTH, CRYSTAL STRUCTURE AND OPTICAL PROPERTIES OF $CdTe_{1-x}Se_x$ THIN FILMS PREPARED BY QUASI CLOSE-SPACE SUBLIMATION METHOD

R. Petrus, H. Ilchuk, A. Kashuba, I. Semkiv, N. Ukrainets
Department of General Physics, Lviv Polytechnic National University, 12, S. Bandera Str., Lviv-79013, Ukraine
e-mail: petrusrom@gmail.com

Thin films of cadmium chalcogenides (CdX, X= S, Se and Te) representative of $A^{II}B^{VI}$ crystal group and shows semiconductor behavior. They are an important research field because of their wide application in various fields of optoelectronic devices [1].

$CdTe_{1-x}Se_x$ (CTS) thin film was prepared by quasi close-space sublimation method. The glass substrates were ~14 mm in diameter were used for deposition CTS thin films. Before the films deposition, the substrate surface was cleaned by boiling in a high purity CCl_4 solution during 0.5 h.

The phase analysis and crystal structure refinement were examined with using X-ray diffraction data. The mean grain size was determined using the Scherrer formula. The strain and the dislocation density are also calculated.

CTS thin film crystallize in cubic structure (structure type –ZnS, space group F-43m, with unit-cell constants a= 6.395(3) Å and V= 261.6(4) Å^3).

Chemical composition of the films was examined using energy dispersive spectroscopy (EDS). The surface morphology of the obtained CTS films was studied using a JSM 6700F scanning electron microscope.

The spectral dependence of the optical transmittance (Shimandzu UV-3600) of the obtained samples in the visible and near infrared regions is studied. The transmission spectra T(λ) of CTS films are characterized by a pronounced edge of the fundamental absorption localized in the vicinity of ~850 nm.

The perspective of research this material is found in forming $CdS/CdTe_{1-x}Se_x$ heterojunction.

[1] R.Yu. Petrus, H.A. Ilchuk, A.I. Kashuba, I.V. Semkiv, E.O. Zmiiovska, R.M. Lys, *Physics and Chemistry of Solid State*, **2019**, 20(4), 367.
[2] R.Yu. Petrus, H.A. Ilchuk, A.I. Kashuba, I. Semkiv, E. Zmiiovska, *Optics and Spectroscopy*, **2019**, 126(3), 220.

STUDY OF THE FORMATION OF GLASS ENAMEL COATINGS PART FOR STEEL PIPES

An. Salei, V. Goleus, T. Kozyreva
Ukrainian State University of Chemical Technology, Gagarin av, 8, Dnipro, 49000, Ukraine
e-mail: saleiandrew@gmail.com

Glass enamel coatings are an effective means of protecting steel pipes from corrosion. These coatings are obtained by slip firing technology using borosilicate glasses, which have a high chemical resistance to the action of various aggressive environments. The protective properties of glass enamels largely depend on the presence of cracks and bubbles. The defectiveness of glass coatings largely depends on the temperature-time regime of their firing. In this regard, the goal of this work is to establish, depending on temperature, the main stages of the formation of anti corrosion coatings for steel pipes based on borosilicate frit [1].

Coatings were applied to the surface of the steel in the traditional slip method. Drying of coatings was carried out at 60-80^{0}C. Samples 5×5 mm in size were placed in a heating microscope furnace [2], with the aid of which the change in coating was visually observed, both in time and with increasing temperature from room temperature to isothermal exposure temperature (860^{0}C), at which coating formation was completed within 10 minutes. As a result of the studies, the following sequence of coating formation was established (Fig. 1).

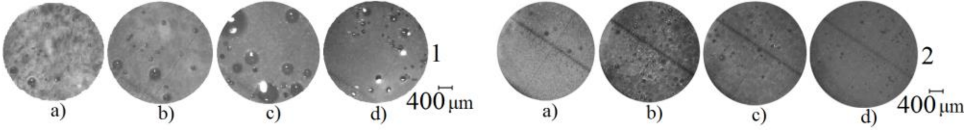


Figure 1 – Stages of coatings formation on steel pipes

At the initial stages of coating formation, sintering and shrinkage of the glass powder are observed at 460-520^{0}C, as well as the formation of a melt at 500-600^{0}C. In compositions with different contents of refractory oxides in the temperature range 640-660^{0}C, bubbles with a diameter of 20-80 μm and 40-60 μm, respectively, are formed (Figs. 1, 1a, 2a). In melts with a high content of refractory oxides with a further increase in temperature up to the calcination temperature, these bubbles increase to d = 100-200 μm and 400-420 μm, and their number increases significantly (Figs. 1, 1b, 1c). By the end of 7 minutes of firing in the melt, only bubbles d = 20-80 μm are observed (Fig. 1, 1d). In melts with a lower content of refractory oxides, after 4-5 minutes of firing, bubbles diameter of 150-170 μm are removed from the melt (Figs. 1, 2b, 2c). During visual inspection of the coating after firing, an insignificant number of bubbles with a diameter of 40-50 microns is observed (Fig. 1, 2d).As a result of the studies, it was found that in enamels with a high content of refractory oxides, the process of clarification of the melt proceeds much more slowly, and the diameters of gas inclusions resulting from firing are larger compared to enamels containing a less of refractory oxides.

[1] Pat. UA 115634 Enamel, Goleus V.I., Kislichna R.I., Kozyreva T.I.., Nagorna T.I., Naumenko S.Yu., Salei An.A., Nikitchuk S.M., № a 201610834, claimed 28.10.16, published 10.07.17, Bul. №13, 4 p.
[2] Goleus V.I. Research of formation of enamel coatings on aluminum, *Physics and chemistry of solid state*. **2014**, V. 15, №3, P. 672-676.

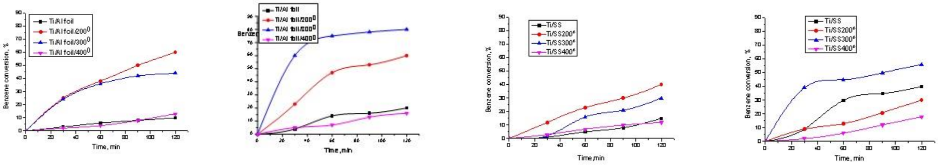
USING Ti-CONTAINING STAINLESS STEEL AND ALUMINIUM FOIL COMPOSITES FOR BENZENE VAPOR PHOTODESTRUCTION

Sanzhak O.V.[1], Brazhnyk D.V.[1], Goncharov V.V.[2], Zazhigalov V.A.[1],
[1] *Departmen of Heterogeneous Catalytic Oxidation Processes, Institute for Sorption and Problems of Endoecology NAS of Ukraine, General Naumov Str., 13, Kyiv-03164, Ukraine.*
E-mail: Sanzhakalena@bigmir.net
[2] *State Establishment, Lugansk State Medical University, Budivelnykiv Str., 32, Rubizhne-93012, Ukraine*

The widespread use of catalytic technologies in industry requires a thorough study of all properties of catalysts. The main requirements for modern catalysts are mechanical strength, thermal stability, activity and selectivity. Catalytic systems deposited on metals and alloys satisfy these requirements. Synthesis of the supported on Aluminium foil and AISI 321 stainless steel foil composites was carried out by low temperature ion implantation method. Ti was used as an implant. The cathode sputtering of the target (Ti) was carried out by N_2 ions. The energy of implantation is 20 keV at a dose of $5x10^{17}$ ions/cm2. The obtained samples were calcinated on air in the temperature range of 200-400 °C. The surface composition and the effect of calcination temperature were characterized by XRD, SAXS, SEM, AFM, and XPS. It was shown that as a result of ion implantation of Ti on the surface of a stainless steel, a nanosized layer of the implant is formed, in the form of amorphous composition consisting of oxide, nitride and titanium oxynitride.

The activity of synthesized samples was determined in the reaction of photodegradation of gaseous benzene (130 threshold limit values (TLV)). The high pressure mercury or sodium lamps were used as a source of radiation. In the case of UV-irradiation samples after treatments at 200 and 300°C have the maximum activity . At visible light irradiation the most active catalysts are the initial implanted sample Ti/SS and Ti/SS300, Ti/Al foil200 and Ti/Al foil300. Further temperature treatment reduces the catalyst photoactivity. Those kinds of changes in samples activity can be explained with influence of temperature on the ratios between nitride, oxynitride and oxide phases of the titanium. The thermal treatment leads to TiO_2 phase formation and it has negative effect on samples properties.

Photodegradation of gaseous benzene



UV Vis UV Vis

THERMAL STABILITY AND VISCO-ELASTIC PROPERTIES OF THE FILMS ON THE BASIS OF EPOXY-OLIGOESTERIC MIXTURES

Olena Shyshchak, Olena Astakhova, Michael Bratychak
Lviv Polytechnic National University, 12 Bandery St., Lviv 79013, Ukraine
e-mail: mbratychak@gmail.com

Oligomers with functional groups based on epoxy resins may be used as active additives for the formation of such products as protective coatings for various solid materials, in particular metal, glass, *etc*. They are resistant to atmospheric and environmental conditions. But in some cases, such coatings are exposed to high temperatures and it is important to know their thermal stability. One more important operation property of protective coatings based on polymer mixtures is their visco-elasticity.

To study thermal stability and visco-elastic properties of the synthesized films we prepared the mixtures of the following compositions:

Component	Component amount, wt parts					
	I	II	III	IV	V	VI
Epidian-5	100	91	60	55	60	55
Oligoester I	–	–	40	36	–	–
Oligoester II	–	–	–	–	40	36
TGM-3	–	9	–	9	–	9
PEPA	14	14	10.6	9	10	9

Notes: Oligoester I was synthesized via the reaction of dioxydiphenylpropane diglycidyl ether + adipic acid in the presence of benzyltriethylammonium chloride; Oligoester II – via the reaction of Epidian-5 + adipic acid in the presence of benzyltriethylammonium chloride. Polyethylenepolyamine (PEPA) served as a hardening agent.

Epoxy-oligoesteric films were prepared by applying a mixture over the standard glass plates. The mixture was prepared as a result of all components mechanical mixing with PEPA hardener. Films were formed stepwise: at first at room temperature for 24 h, and then at 423 K for 75 min.

By means of TGA analysis it was established that oligoester I is a sufficiently stable product up to the temperature of 433 K. Epidian-5 based films with oligoester I in their composition are completely decomposed at 873 K.

The introduction of the synthesized oligoester II into epoxy-oligoesteric mixture improves the visco-elastic properties of the films based on Epidian-5. Films containing oligoester II, in comparison with Epidian-5-based films without oligoester II, are characterized by better homogeneity and restorability.

ELECTRO- AND PHOTOELECTROPHYSICAL PROPERTIES OF NEW PHOTOSENSITIVE THIN FILM STRUCTURES BASED ON ANIONIC σ-COMPLEXES

Studzinsky S.L.[a], Siniugina A.T.[b]
[a] *Faculty of Chemistry, Macromolecular Chemistry Department, Taras Shevchenko National University of Kyiv, 60 Volodymyrska Street, Kyiv, 01033, Ukraine.*
[b] *Institute of High Technologies, Taras Shevchenko National University of Kyiv, 60 Volodymyrska Street, Kyiv, 01033, Ukraine.*
e-mail: studzs@ukr.net

The colored anionic sigma complexes – dinitro and trinitro substituted aromatic alkoxyl Meisenheimer complexes – were synthesized by the interaction of 1-chloro-2,4-dinitrobenzene and(or) picryl chloride with corresponding sodium alcoholates. The novel photosensitive thin film structures based on these anionic sigma complexes and their composites with dielectric polymer matrices have been prepared. Their spectral, electric and photoelectrophysical properties have been investigated. All obtained thin film structures are characterized by a high level of ionic conductivity. It was shown, that all studied film structures exhibit photovoltaic effect and photoconductivity under illumination by light from the long-wavelength edge of the synthesized anionic σ-complexes absorption region. The features of electrophysical, photophysical and photoelectric properties of the obtained thin film structures, as well as the possible nature of the photovoltaic effect and charge carriers photogeneration mechanisms are discussed. The respective phenomenological model for internal photoeffect and photovoltaic effect in the investigated thin film structures was proposed.

SYNTHESIS OF LANTHANUM COBALTITE FROM ACETYLACETONATE COMPLEXES $LaCo(AA)_5 \cdot nD$

L.I. Sliusarchuk, L.I. Zheleznova, T.V. Pavlenko, O.O. Rogovtsov, O.K. Trunova
V.I. Vernadsky IGIC NAS Ukraine, 32/34, Palladin Avenue, 03142, Kyiv -142, Ukraine
e-mail: l.sliusarchuk@yahoo.com

The heterometallic acetylacetonate complexes $LaCo(AA)_5 \cdot nD$ (AA – acetylacetonate, D - H_2O, αα'-dipyridyl (αα'-dipy)) have been synthesized as precursors for the obtaining of heterometallic oxide structures. The complexes are characterized by electronic absorption spectra and IR spectroscopy and X-ray powder diffraction. Their thermal stability was studied. The experiments with changing the thermolysis conditions, namely, varying the heating rate (from 5 °C/min to 20 °C/min), changing the final heating temperature (up to 500 °C and up to 800 °C), and holding time at the final temperature (from 1 to 5 hours) were conducted to develop a method for thermolysis of heterometallic complexes. The control of the composition of the obtained oxide powders after heat treatment was carried out by X-ray powder diffraction.

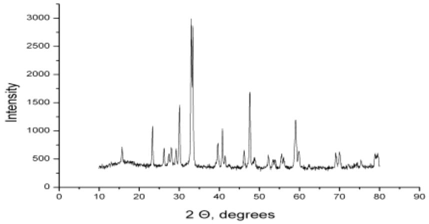


Figure X-ray powder diffraction pattern of – $LaCo(AA)_5 \cdot n$(αα'-dipy).

In the **Figure** it shows the diffraction pattern of the sample $LaCo(AA)_5 \cdot n$(αα'-dipy). The conditions of synthesis were the heating at a rate of 20 °C/min and the keeping at 700 °C for three hours. The final product of thermolysis in air is a single-phase crystalline powder - monoclinic lanthanum cobaltite ($LaCoO_3$) with parameters of the cell: a = 5.3611 Å, b = 5.4316 Å, c = 7.6318 Å, β = 91.056 º and traces of La_2O_3 were also fixed in the spectrum, according to the data of X-ray powder diffraction. In the case of thermolysis of a mixture of monocomplexes ($La(AA)_3 \cdot nH_2O$ and $Co(AA)_2 \cdot nH_2O$) along with the formation of a complex oxide, the data of X-ray powder diffraction showed the presence of lanthanum oxide (La_2O_3) and cobalt oxide (Co_3O_4), and their percentage is much higher than at pyrolysis of heterometallic acetylacetonate complexes.

The possibility of obtaining lanthanum cobaltite from a heterometallic precursors $LaCo(AA)_5 \cdot nD$ is shown.

PHOTOELECTROCHEMICAL PROPERTIES OF COPPER VANADATE

V.O. Smilyk[1], S.S. Fomanyuk, G.Ya. Kolbasov, I.A. Rusetskii
[1] *V.I. Vernadskii Institute of General and Inorganic Chemistry of the Ukrainian NAS, prospekt Palladina 32–34 Kyiv 03142, Ukraine*
e-mail: VitaliySmilyk@i.ua

The efficient conversion of solar energy into chemical fuel using stable semiconductor photoelectrodes has been the subject of intense research over the last several decades in the field of photoelectrochemistry. It should be noted that almost 50% of the incident solar energy on the Earth's surface falls within the energy range of visible light, so recent studies have focused on the synthesis and development of n-type and p-type metal oxide photoelectrodes capable of absorbing visible light. One of such materials is Cu_3VO_4, because the position of its conduction band lies in the range of water decomposition potentials [1]. Therefore, Cu_3VO_4 may be a promising cathode photoelectrode for hydrogen evolution. In addition, copper vanadate has a fairly high resistance to photocorrosion. The Cu_3VO_4 photocathode was obtained by electrochemical deposition of V_2O_5 films followed by sintering with Cu_2O under argon. V_2O_5 films were obtained at a cathode current of 1- 0.5 mA / cm^2) from an electrolyte based on $VOSO_4$ − 7 g/l and CH_3COONH_4 − 0.154 g/l, with a pH of 4.85 which was brought about by the addition of nitric acid (HNO_3). Cu_2O on the surface of V_2O_5 was applied by spraying a solution of 35 g/l Cu $(NO_3)_2$ in 30% ethyl alcohol. The dried samples were then air-dried and annealed in argon at 450°C.

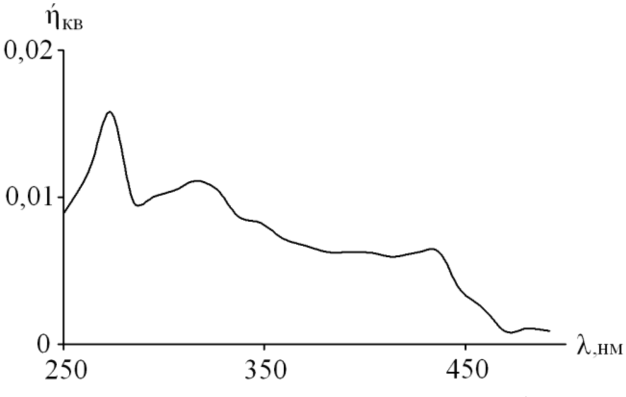


Fig. 1 Quantum output spectrum of Cu_3VO_4 film photocurrent at -0.2 V Rel. hp

Figure 1 shows the quantum output spectrum of the Cu_3VO_4 photocurrent. As can be seen, photocurrent is observed over a wide range of wavelengths. Spectrum analysis showed that the obtained p-Cu_3VO_4 semiconductor material has a bandgap of Eg = 2.5 eV, so it can be used in conjunction with a photoanode based on n-$BiVO_4$ (Eg = 2.4-2.6 eV) for photoelectrochemical water decomposition.

[1] C. W. Lee, H. K. Park, S. Park, Mater. Chem. A, **2015**, 3, 825–831.

PHOTOELECTRET PROPERTIES OF PHOTOSENSITIVE POLYMERIC COMPOSITES DOPED BY TRIARYLMETHANE DYES

Studzinsky S.L.
Faculty of Chemistry, Macromolecular Chemistry Department, Taras Shevchenko National University of Kyiv, 60 Volodymyrska Street, Kyiv, 01033, Ukraine.
e-mail: studzs@ukr.net

The photosensitive thin film polymeric structures based on non-photoconducting or photoconducting polymer matrices doped by various concentration of triarylmethane and xanthene type dyes have been prepared. Their spectral and electro- and photophysical properties have been investigated. It was shown, that studied composite films exhibit photoelectret effect without external polarizing field under illumination by light from the dye absorption region. The results of investigation of the photoelectret state in these film composites are presented. The features of the photophysical and photoelectret state properties of the investigated film compositions, as well as the possible nature of the photoelectret effect and charge carriers photogeneration mechanisms are discussed. The phenomenological model for internal photoeffect and photoelectret effect in investigated compositions was proposed.

EFFECT OF NANOSTRUCTURING TO RESPONSE KINETICS OF TELLURIUM THIN FILMS BY NITROGEN DIOXIDE SENSING

Dumitru Tsiulyanu[a], Marina Ciobanu, Olga Mocreac
[a] *Department of Physics, Technical University, bul. Dacia 41, MD-2060 Chisinau, Moldova,*
tsiudima@gmail.com

The work is conducted to clarify the effect of structural dimensionality of tellurium thin films on gas (NO_2) sensing at room temperature. Nanostructuring of Te films has been realized via three methods (Fig.1): nanocrystalization (a), growing of amorphous Te films with nanoscaled thicknesses onto uniform Si/SiO_2 wafers (b) or onto priory nanostructured (Al_2O_3) substrates (c). Pure Te thin films were crown via thermal vacuum evaporation but their surface morphology, microstructure and thickness were investigated using SEM, XRD and AFM respectively. The films were supplied with either Au or Pt electrodes, thus the resistive gas sensing elements have been built. Their gas sensing properties have been investigated using the experimental set-up described in [1], taking into consideration the concentration induced damping of gas sensitivity in ultrathin layers found out in our previous work [2].

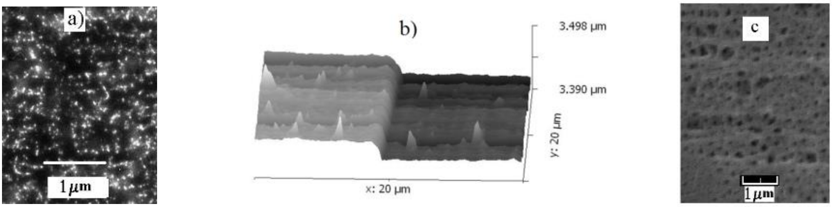


Fig.1. (a) SEM of nanocristalline Te film; (b) AFM of an ultrathin amorphous Te film; (c) SEM of an amorphous Te film grown onto preliminary nanostructured substrate.

It was shown that the response kinetics of tellurium thin films is strongly influenced by structural dimensionality, which is controlled by grown rate. The increasing of growing rate results in transformation of nanocrystalline structure of the film into an amorphous one. Amorphous films, being nanoscaled either by diminishing the films thickness or by their growing onto preliminary nanostructured substrates, show considerably short response time to low concentrations of nitrogen dioxide. The recovery time of initial state of these films, also become shorter that allows their application in development of room temperature operating gas sensitive devices for environment pollution monitoring.

[1] D. Tsiulyanu, M. Ciobanu, Glass Physics and Chemistry, **2019**, 45, pp. 53–59.
[2] D. Tsiulyanu, O. Mocreac, Sensors and Actuators , B, **2013**, 177, pp. 1128 – 1133.

PHOTOTHERMOPLASTIC RECORDING MEDIA AND ITS APPLICATION IN THE HOLOGRAPHIC METHOD OF DETERMINATION OF REFRACTIVE INDEX OF LIQUID AND GASEOUS OBJECTS

Studzinsky S.L.[a], Pavlov V.A., Chuprina N.G., Kuranda N.N., Mokrinskaya E.V., Kravchenko V.V., Davidenko N.A, Davidenko I.I.
[a] *Faculty of Chemistry, Macromolecular Chemistry Department, Taras Shevchenko National University of Kyiv, 60 Volodymyrska Street, Kyiv, 01033, Ukraine.*
e-mail: studzs@ukr.net

The photothermoplastic medium based on the films of photosensitive polymeric composites with semiconductor properties is developed for application in optical information recording and storage, in holographic interferometry as well as for medical purposes. The present work is aimed at creation of new cooligomer providing higher diffraction efficiency when it is used as the holographic recording media (HRM) base for photothermoplastic (PTP) holographic recording as well as at employing these HRM for determination of the refractive index of the liquid and gaseous objects. Cuvette without diffuser and reversible holographic medium without “wet” development of the holograms were used. With the aim to increase the precision of measurements of the refractive index, the method of phase steps (Phase Shifting Interferometry) of analysis of the interferograms was applied. This medium was used in the modified holographic device for determination of the refractive index of homogeneous and inhomogeneous liquid and gaseous objects. To reach the aim of the present work, above described HRM were used for determination of the refractive index (n) of liquid and gaseous objects. The method includes transmission of the coherent irradiation through trapezoidal cuvette alternately fillable with standard and investigated media, registration of the hologram, its reconstruction and determination of the n value by measurement of the spatial frequency of interference strips using Phase Shifting Interferometry. For determination of the refractive index n equipment schematically shown in Fig.1 was used.

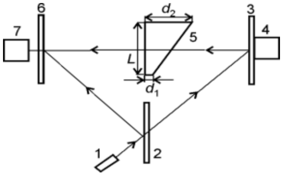


Fig. 1. Optical scheme of the small sized holographic equipment (Fig.4): 1 – laser, 2 – light splitter, 3 – mirror, 4 – piezo element, 5 – trapezoidal cuvette with high L and cross-section of planes d_1 and d_2, 6 – HRM, 7 – camera.

The technique and holographic equipment were modified by employing the specially developed and produced transparent cuvette of special shape. Method of “phase steps” was used for the interferograms processing. Experimentally demonstrated precision of the measurements is not less than 10^{-5}.

CRITICAL CURRENT IN HIGH-Tc SUPERCONDUCTOR BICRYSTALS WITH LOW-ANGLE [001]-TILT GRAIN BOUNDARIES

A.L. Kasatkin, V.P. Tsvitkovskyi[a]
[a]*G.V.Kurdyumov Institute of Metral Physics, NAS of Ukraine, 36 Vernadsky blvd, 03142 Kiev, Ukraine*
e-mail: tsvad55@gmail.com

High-temperature superconducting materials (HTS) produced on the base of 'cuprate' compounds (RE)-Ba-Cu-O (RE – is the rare-earth element: Y, Gd, Nd) are of great practical interest for electrical engineering and electronics [1]. This interest is caused by a large current carrying ability of HTS materials, allowing dissipation-free current flow with densities more than 10^6 A/cm^2 at liquid nitrogen temperature (77K) and magnetic fields up to 10 T, obtained for HTS $(RE)Ba_2Cu_3O_{7-\delta}$ ((RE)BCO) films and coatings.

One of the most important structural features of these superconductors, which provides limitations on their current-carrying capability, is existence of grain boundaries (GB) within the material, playing the role of barriers for supercurrent flow [1,2]. For HTS epitaxial thin films and highly textured coatings, which possess the highest j_c values and are mostly interesting for applications, the main type of GB, affecting the critical current value, are [001] – tilt grain boundaries. Experiments performed on [001]-tilt YBCO bicrystals with a single GB of this type have demonstrated that the critical current density across the grain boundary depends strongly on the misorientation angle θ of grains, and drops nearly exponentially when θ increases: $j_c(\theta) \sim exp(-\theta/\theta_c)$ where $\theta_c \approx 2 - 3^0$ [3]. It's well known, that low-angle [001]-tilt GB in YBCO bicrystals and *c*-oriented epitaxial films (coatings) may be considered as rows parallel to the *c*-axis edge dislocations [3]. In this case the current passes the GB through the nano-sized channels between dislocation cores, which are non-superconducting (dielectric or normal-metal cylindrical regions) owing to dislocation cores and strain fields around them.

In the present work the depinning critical current for periodic pinning potential created by a dislocation row along the [001]-tilt low-angle GB (LAB) in HTS bicrystal is calculated. The strong exponential $j_c(\theta)$ dependence for the critical current density is obtained for $\theta \geq 3^0$ at low magnetic field values (e.g., those induced by a transport current). The calculated $j_c(\theta)$ dependence matches quantitatively well with the corresponding experimental data, obtained for YBCO bicrystals.

[1]D. Larbalestier, A. Gurevich, D.M. Feldmann, and A. Polyanskii, *Nature* , 2001, **414**, 368-377.
[2]J.H. Durrell and N.A. Rutter, *Supercond. Sci. Technol.*, 2009, **22**, 013001(1-18).
[3]H. Hilgenkamp and J. Mannhart, *Rev. Mod. Phys.*, 2002, **74**, 485-549 .

CATALYTIC PROPERTIES OF CoRe AND CoWRe ALLOYS IN THE HYDROGEN ELECTROREDUCTION REACTION

T. Maltseva, Yu. Yapontseva, V. Kublanovsky
V. I. Vernadskii Institute of General and Inorganic Chemistry of the Ukrainian NAS,
pr. Palladina 32/34, 03142 Kyiv, Ukraine
e-mail: kublanovsky@ionc.kar.net

Electrolytic coatings with superalloys - alloys of refractory metals (tungsten and rhenium) with metals of the iron subgroup possess a number of unique mechanical and physicochemical properties, such as high corrosion resistance, hardness, wear resistance, heat resistance, magnetic properties, as well as electrocatalytic activity in the hydrogen evolution reaction [1].

It is known that CoW alloys exhibit high electrocatalytic activity in the hydrogen electroreduction reaction. It is of interest to study the effect of the Re content on such electrocatalytic properties of coatings by CoRe and CoWRe alloys deposited from citrate (Cit) and citrate-pyrophosphate (Cit-PPi) electrolytes. The composition of electrolytes, mol/l: $CoSO_4\cdot 7H_2O$ - 0.1; $Na_2SO_4\cdot 10H_2O$ - 0.3; $Na_3C_6H_5O_7\cdot 10H_2O$ - 0.2; $KReO_4$ - 0.01; ($K_4P_2O_7$ – 0.2; $Na_2WO_3\cdot 2H_2O$ – 0.2 - optionally). Coatings were deposited at current density of 30 $mA\cdot cm^{-2}$. The study of electrocatalytic activity was carried out in 1M solution of KOH. To estimate the effect of refractory metals on properties of coatings, the data for electrolytic cobalt is shown on the figure 1. Based on voltammetric studies, the coefficients of Tafel equation and the hydrogen exchange current were determined.

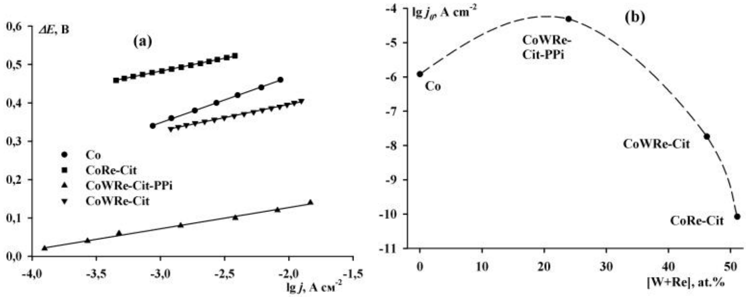


Fig. 1. Linear parts of the Tafel dependencies (a) and the current density of hydrogen exchange for Co and CoRe, CoWRe alloys (b).

It was shown that, unlike cobalt, where charge transfer is the limiting stage (b = 0.119), a mechanism with a limiting stage of electrochemical desorption (b = 0.055 ÷ 0.068) is realized on the alloys under investigation. The highest value of exchange current is observed for coatings containing ~ 20 at.% of refractory components.

[1] V. S. Kublanovsky, Yu S. Yapontseva, Chapter 5 in *"Electrocatalysts for Fuel Cells and Hydrogen Evolution - Theory to Design"* **2018** IntechOpen 95-117.

THIN-FILM STRUCTURES BASED ON Ge - GeO_2 - B_2O_3 AND Ge - ZnS (ZnO) - B_2O_3 SYSTEMS FOR INTERFERENCE OPTICS OF IR SPECTRUM RANGE

V. Zinchenko[1], I. Magunov[1], O. Mozkova[2], G. Volchak[1]
[1]O.V.Bogatsky Physico-Chemical Institute of NAS of Ukraine,
86 Lustdorfska Doroga Str.Odesa 65080, Ukraine,
e-mail: vfzinchenko@ukr.net
[2]State Enterprise for Special Instrument Making "Arsenal",
8, Moscovska Street, Kyiv 02010 Ukraine
e-mail: borisgor@ukr.net

Interference optics consists of alternating thin layers of substances with different refractive indices deposited on a substrate of a certain material [1].

In recent years, we have developed a new type of coating materials - composites of the composition Germanium – metal chalcogenide (oxide), capable of congruent evaporation in vacuum. On the other hand, B_2O_3 serves as an effective additive to stabilize the evaporation process in some systems. Boron oxide reacts with the oxide components of the systems to form fairly strong compounds. This is especially pronounced in the case of ZnO, forming several compounds according to the scheme:

$$mZnO + nB_2O_3 \rightarrow Zn_mB_{2n}O_{m+3n}. \qquad (1)$$

In the Ge-GeO_2-B_2O_3 system, Germanium as could not be identified borate-type compounds due to glass formation. The formation of very strong compounds (borates) prevents the admixture of Zinc oxide from interacting with the evaporator material when applying ZnS and Ge-ZnS coatings containing B_2O_3 additive. This makes possible to obtain very strong coatings with noticeably different refractive indices (2.3 and 3.0), which are successfully used in the interference optics of the IR spectral range.

Additive B_2O_3 has been shown to be effective in producing a GeO film on a germanium substrate from the Ge-GeO_2-B_2O_3 system. Due to chemical interaction in the system, the evaporation process proceeds in a quiet technological mode, resulting in a uniform coating with good adhesion to the substrate. The use of the described composites opens up the possibility of obtaining optical elements with interference coatings of the IR spectral range, which have high operational and optical parameters.

[1] Bubis I.Ya., Veidenbackh V.A., Dukhopel I.I. et al. Handbook on optics / Ed. Kuznetsov S.M. and Okatov M.A. Leningrad: Mashinostroenie, 1983. −414 p.

THE PRECONCENTRATION OF AROMATIC ALDEHYDES ON POLYDIMETHYLSILOXANE-DIVINYLBENZENE FIBER

A.O. Mosendz, V.M. Levchyk, M.F. Zui
Taras Shevchenko National University of Kyiv,
64/13, Volodymyrska Street, Kyiv 01601, Ukraine
e-mail: nastia13mosendz@gmail.com

Solid-phase microextraction is a modern method of sample preparation in chemical analysis which allows to separate analytes from the complex matrix and to preconcentrate them. The main advantages of the method are environmental friendliness and ease of execution. Solid-phase microextraction is based on the sorption of the analyte into a thin layer of coating on a fiber fixed in a special device and subsequent thermal desorption in a injector of chromatograph. The dimensions of the typical SPME fiber coatings are 1 cm long and less than or equal to 100 μm thick.

The point of our study was to preconcentrate aromatic aldehydes from aqueous samples. The properties and content of various aldehydes can be different. In particular, formaldehyde and acrolein, even in small quantities, are harmful, undesirable components, but some amounts of aromatic aldehydes, such as benzaldehyde, are found in teas and stipulate their aroma and quality. Therefore, the level of certain aldehydes can be used to control the undesirable compounds or determine the quality of food and beverages.

A derivatization of the aldehydes prior to preconcentration was required to increase the sensitivity of chromatographic determination.

Supelco commercial fibers were used in this study. According to the literature, the polydimethylsiloxane-divinylbenzene fibers are most suitable for the recovery of volatile compounds with medium molecular size. These fibers have following parameters: thickness 65 μm, surface area 750 m^2/g, total porosity 1.54 ml/g, phase volume 0.44 μl, stability up to 270 °C, pH range 2-11 [1].

The optimum parameters affecting the extraction are determined: sorption time of 30 min, sorption temperature of 60 °C, content of salting-out agent (NaCl) 10%. Also the conditions of derivatization were selected: pH 4.0; derivatization time 20 min. Benzaldehyde and 2,4-dimethylbenzaldehyde were identified in tea samples, 2-furaldehyde – in coffee sample and 4-methoxybenzaldehyde – in aqueous model solutions. Quantitative characteristics of microextraction and chromatographic determination of the compounds were defined. The detection limits (signal-to-noise ratio of 3) are 19 – 25 μg/L.

[1] J. Pawliszyn. Handbook of Solid Phase Microextraction.. London: Elsevier. – 2012. – 496 p.

SECTION 4

ELECTRONIC PROCESSES IN NANOSTRUCTURES AND POLYMER COMPOSITES

FEATURES OF RAMAN SCATTERING AND X- RAY DIFFRACTION IN As-Se-Te(S) CHALCOGENIDE GLASSES DOPED BY SAMARIUM

R.I. Alekberov[a,b], A.I. Isayev[a], S.I. Mekhtiyeva[a]
[a] Institute of Physics named after academician G.M. Abdullayev's of Azerbaijan National Academy of Sciences, G. Javid ave 13, AZ1143 Baku, Azerbaijan Phone: (+994 12) 539-35-28, Fax: (+994 12) 5395961,
Email: rahim-14@mail.ru
[b]Azerbaijan State University of Economics (UNEC), st. Istiqlaliyyat 6, Baku, AZ 1001

Chalcogenide glassy semiconductors are promising materials for application in electronics and optoelectronics [1]. For this purpose, it is necessary to find methods to control their electronic properties. Glass-like and amorphous semiconductors contain nanometer-size in homogeneities, in which there is a certain order in the arrangement of structural elements. These in-homogeneities are not isolated entities, but are fragments of which are built entirely amorphous and glassy matters, i.e. they may be considered analogous to the crystal unit cell [2]. Information about these fragments give experiments on neutron diffraction [3] or X-rays [4], as well as the observable features in low frequencies in the Raman spectrum of such materials [5].Raman spectra of amorphous and glassy materials differs from that of the corresponding crystals so that they plot in the low frequency ($\omega < 100$ cm^{-1}), there are two features: the boson peak (BP) and quasi-elastic scattering. BP is associated with the existence of excess density of states of acoustic vibrations localized in-homogeneities in the material [2].

The structure of chalcogenide glassy semiconductors (CGS) $As_{33.3}Se_{33.3}S_{33.4}$, $As_{33.3}Se_{33.3}Te_{33.4}$ and the influence on them of samarium additives have been studied by method of X-ray diffraction and Raman scattering (RS) of light. The observed peculiarities of the diffraction picture are explained by the Elliott void-cluster model. The structural parameters of CGS materials $As_{33.3}Se_{33.3}S_{33.4}$, $As_{33.3}Se_{33.3}Te_{33.4}$ with and without impurities of samarium are determined. It has been established that the Raman spectrum CGS materials $As_{33.3}Se_{33.3}S_{33.4}$, $As_{33.3}Se_{33.3}Te_{33.4}$at frequencies below 100 cm^{-1} consists of two parts: first - which the intensity with increasing frequency up to 30 ÷ 40 cm^{-1} decreases (quasi-elastic scattering); second - which have been observed a broad band with a maximum at frequencies of ~ 63 ÷ 67 cm^{-1} (boson peak - BP). Such a case is absent in the respective crystals. The observed features are associated with structural relaxation and excess density of states of acoustic vibrations in irregularities is localized with nanometer-size of material.

[1] A. V. Semencha, M.V.Kurushkin, V. A. Markov, Moisture resistance of the As-S-I glasses. Advanced Materials Research. vol.1061-1062(2015)987-990.
[2] V.K. Malinovski, FTT, 41(1999)805
[3] G. Swenson, R. L. McGreevy, L. Borjesson , J. D. Wicks, W. S. Howells, J. Phys.: Cond. Matter. 8(1996)3445
[4] R.I. Alekberov, A.I. Isayev, S.I. Mekhtiyeva,G.A.Isayeva,Chalcogenide Letters,10(2013)335-339 [5] A. Fontana, G. Mariotto, E.Gazzanelli, G. Carni, M. Cutroni, M. Federico. Phys.Lett. A93, 4, 209(1983)

INFLUENCE OF GAMMA RADIATION ON THE ELECTRICAL PROPERTIES OF EXTRUDED SAMPLES OF SOLID SOLUTION $Bi_{85}Sb_{15}$ <Te>

Abdullayeva I.A. [1,2], Abdinova G.D.[2]., Tagiyev M.M.[3.2]
[1]*Institute of Radiation Problems of NAS of Azerbaijan, Baku, B. Vapabzadeh str., 9*
[2]*Institute of Physics of National Academy of Sciences of Azerbaijan, Baku, H. Javid Ave. 131,*
[3]*Azerbaijan State Economic University, Baku, Isiglaliyyat str.6.*
Email: mail_tagiyev@mail.ru

Solid solutions of Bi-Sb systems are promising materials for the creation of low-temperature thermo- and magnetothermoelectric converters. Particularly promising in this direction are high-strength extruded materials based on these systems. These devices are often used in radiation conditions. Therefore, the study of the effect of radiation defects on the electrical properties of Bi-Sb systems acquires a certain scientific and practical interest.

In order to clarify the peculiarities of the influence of radiation defects on the electrical properties of solid solutions of Bi-Sb systems, extruded $Bi_{85}Sb_{15}$ samples doped with 0.0005 at. % Te were obtained and their electrical properties were studied depending on the dose of gamma-radiation in the temperature range ~77 ÷ 300 K.

Samples were irradiated with gamma-rays (gamma-radiation) in ^{60}Co isotope source with different doses (1; 10 and 50 Mrad). We studied the electrical conductivity (σ), the coefficients thermo-emf (α) and Hall (R_H) of the samples, as annealed after extrusion, and the same samples irradiated with gamma rays at various doses. It was found that, in non-doped samples with an increase in the radiation dose of the samples, the carrier concentration decreases, and the mobility increases in the entire studied temperature range, except for the sample irradiated with gamma-rays with a dose of 1 Mrad. At low radiation doses (1 mrad), the concentration of current carriers (n) in the samples slightly increases, and the mobility (μ) decreases. As the radiation dose in the samples increases, n decreases significantly, and μ grows. These changes in n and μ correlate well with changes in σ and α. In non-irradiated samples doped with 0.0005 at.% Te, the concentration of charge carriers is lower than in samples irradiated with various doses of gamma-rays. In the $Bi_{85}Sb_{15}$ <Te> sample irradiated with gamma-quanta with a dose of 1 Mrad carrier concentration is higher than in other doses of irradiation with gamma quanta.

During extrusion due to plastic deformation, structural defects, which are scattering centers for current carriers, are formed in the samples in parallel with the texture formation. At the same time, the concentration of current carriers also increases. Tellurium atoms in the samples create donor centers. In non-doped samples, the insignificant effect of gamma-radiation on α with a significant change in σ shows that upon irradiation, mainly, the mobility of charge carriers changes, i.e. the concentration of scattering centers for electrons decreases. A small change in α at irradiation with gamma-quanta indicates that the defects formed during plastic deformation are mainly non-ionized. In samples doped with tellurium atoms 0.0005 at.% a significant effect of gamma-radiation on α and σ shows that radiation defects playing the role of donor centers increase concentration of charge carriers.

EXCITONIC EFFECTS IN AGGREGATES OF ORGANIC DYES AND CARBONIC NANOSTRUCTURES

Alexander P. Demchenko[a,b]
[a] *Palladin Institute of Biochemistry, Leontovicha st. 9, Kyiv 01030, Ukraine*
[b] *Yuriy Fedkovych National University, Chernivtsi, 58012, Ukraine*
e-mail: alexdem@ukr.net

When organic dyes are assembled into nanostructures, their properties change dramatically. Some of them form well-ordered H- and J-aggregates, in which their photophysics behavior changes from molecular to excitonic. Generation of Frenkel-type small-radius excitons in J-aggregates modifies dramatically the absorption and emission spectra. The spectra become extremely narrow, shifted to longer wavelengths, without signature of vibronic structure and with very small Stokes shifts. Propagating excitons generate such effects as “superradiance”, “supernarrowing” and “superquenching”. The most efficient J-aggregate formers are the cyanine dyes that spontaneously assemble in water.

In contrast, H-aggregates demonstrate broad absorption and emission spectra with strong Stokes shifts. Many dyes can form non-emissive H-dimers causing self-quenching in molecular ensembles. However, they can be brightly fluorescent in some cases.

The molecular dimer model of Michael Kasha and its extensions can adequately explain these excitonic properties and provide the background for application of dye aggregates in photovoltaics and also in chemical and biological sensing.

The recently discovered fluorescent nanoparticles made of inorganic carbon (C-dots) have rapidly found broad range of applications, particular in molecular sensing and cellular imaging. The origin of their bright emission is not well established and is a subject of active discussion. Based on results of structural, spectroscopic and single-molecular studies the excitonic nature of their photophysical behavior was suggested. This concept will be discussed presenting systematic analysis of experimental data.

THE NATURE OF OVERTONES AND COMBINATIONS OF FUNDAMENTAL VIBRATIONAL MODES IN RAMAN SCATTERING SPECTRA OF LEAD PHTHALOCYANINE FILMS

M.P.Gorishnyi, O.M.Fesenko

Institute of Physics, National Academy of Sciences of Ukraine
Prospect Nauki, 46, 03208, Kyiv, Ukraine
e -mail: miron.gorishny@gmail.com

The structure, absorption and Raman scattering spectra of lead phthalocyanine (PbPc) films with a thickness 185nm were investigated. These films were obtained by thermal spraying in a vacuum of 6.5 mPa on quartz substrates. The structure of these films was investigated by optical and electron microscopy methods. The Raman scattering spectra of PbPc films are shown in Fig.1 in spectral regions of 100 – 2970 cm^{-1} (a) and 1680 – 2970 cm^{-1} (b).

It is established, that the structure of PbPc films is formed by crystallites of monoclinic and triclinic modifications and amorphous phase, which are formed during the vacuum thermal deposition of these films on quartz substrates. Raman bands in the spectral region (1680 - 2970) cm^{-1} were first interpreted as overtones or combinations of fundamental vibrational modes of PbPc from the region (100 - 1680) cm^{-1}. However, the relative peak intensities of overtones and combinations are much smaller than those for the fundamental vibrational modes that form them.

Breathing vibrational modes of macrocycle, benzene rings and pyrrole rings of PbPc molecule were observed with frequencies 674.2; 938.9 and 1138.0 cm^{-1} respectively. Of these, the first two intense vibrational modes are active. They combine with local fundamental vibrational modes, caused by bending of the C-H -bonds and the C=C -bonds of the pyrrole rings and the C-N -bonds of the azo-groups.

It is established, that the most active are the local fundamental vibrational modes 1339,1 and 1449,8 cm^{-1}, which are caused by stretches the C=C -bonds of the pyrrole rings and the C-N -bonds of the azo-groups respectively. Of these, the first vibrational mode forms eleven, and the second vibrational mode - ten combinations with different fundamental vibrational modes respectively.

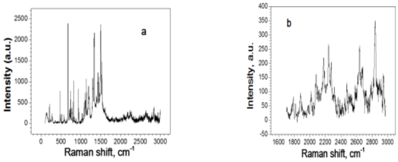
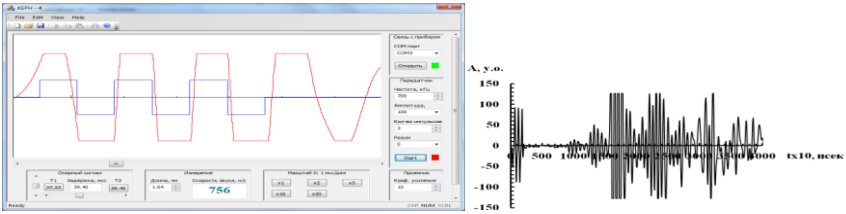


Fig.1. Raman scattering spectra of PbPc films

PECULIARITY OF INELASTIC CHARACTERISTICS OF NANOCOMPOSITES MULTIWALLED CARBON NANOTUBES AND POLYETHYLENE, POLYVINYL CHLORIDE, POROUS POLYSTYRENE, RADIATION CROSS-LINKED HYDROGELS

A.P. Onanko, M.P. Kulish, Y.A. Onanko, N.V. Kutsevol, O.N. Nadtoka, D.V. Charnyi, O.P. Dmytrenko, T.M. Pinchuk-Rugal, M.A. Aleksandrov, O.L. Pavlenko, T.O. Busko, P.P. Ilyin, O.M. Rozhkovskiy
Taras Shevchenko Kyiv national university, Volodymyrs'ka str., 64, Kyiv 01601, Ukraine
e-mail: onanko@i.ua

The quasitransversal ultrasonic (US) velocity V⊥ = 756± 10 m/sec, shear module G = $\rho V_{\perp 1}^2$ = 554 MPa, Puasson coefficient $\mu \approx 0{,}44$ and Debye temperature $\theta_D \approx 71$ K of the polyethylene with low density high pressure $(C_2H_4)_n$ were determined from the oscilloscopegramma on fig. 1 [1]. The US attenuation logarithmic decrement was $\delta_\perp \approx 1{,}65 \times 10^{-1}$.



Частота, кГц 700
Амплитуда 100
Длина, мм 1.64
Скорость звука, м/с 756

Figure. 1. The window illustration of data treatment of quasitransversal elastic waves velocity measuring V⊥ = 756 ± 10 m/sec and the oscilloscopegramma of impulses in the nanocomposite polyethylene with low density high pressure $(C_2H_4)_n$ + 0,2% multiwalled carbon nanotubes by impulse-phase method at frequency f⊥ = 0,7 MGz.

Conclusion

The concentration C = 5% of the polyvinyl alcohol radiation cross-linked hydrogel with the maximal absolute values of the static module E(C) at compression and at extension; elastic limit $\sigma_E(C)$; effective fluidity limit $\sigma_{fl}(C)$; strength limit at compression $\sigma_{st}(C)$ were discovered in consequence of the formation of the polyvinyl alcohol molecules nanoclusters.

References

[1] A.P. Onanko, O.V. Lyashenko, Y.A. Onanko, *J. Acoust. Soc. Am.*, **2008**, 123, № 5, Pt. 2, 3701.

MANIFESTATION OF THE SPECIAL NANO-STRUCTURAL PROPERTIES OF LAYERED TRANSITION METAL DIHALCOGENIDES AND GRAPHENE WITH CHANGE IN THE NUMBER OF MONO-LAYERS

Kornienko N.E., Naumenko A.P., Gubanov V.O.
Taras Shevchenko National University of Kyiv, 64/13 Volodymyrska Str., 01601 Kyiv,Ukraine
e-mail: nikkorn@univ.kiev.ua

Based on a large amount of experimental material on Raman spectra (RS) of a wide range of layered transition metal dichalcogenides (TMD) (MoS_2, WS_2, WSe_2, $MoTe_2$, etc.) and graphene both from our own measurements and borrowed from the literature [1,2] a systematic analysis of the dependences of the intensities of the vibrational bands (VB) A_{1g}, E_{2g}, G, D, 2D, and others on the number of monolayers I(n) was performed. The I (n) dependences are compared for a number of VBs excited by various lasers. It is significant that the values of I(n) reach their maxima, which are 2–5 times higher than the values for bulk samples $I\infty$ at n = 2–15. In some publications, these intensity anomalies in RS were explained by interference effects in SiO_2/Si films (~100 - 300 nm), on which layers of TMDs or graphene were fabricated [1, 2]. However, in free films, the VB intensities were often several times higher than the intensities in RS for nanofilms on substrates. Anomalies were observed for the VB frequencies and the ratios of anti-Stokes and Stokes components in RS, as well as for broadband backgrounds, which is not associated with interference. Moreover, for different MoS_2 samples, the I(n) maxima for VB A_{1g} and E_{2g} at 532 nm are observed at different values of n (2, 3, 5-7, or 15), which clearly indicates a change in the properties of layered nanostructures. It should be noted that for a small number of monolayers (n = 1-5), the applicability of the macroscopic approach and the approximation of a continuous medium is limited and the molecular structure must be taken into account.

For the first time, we consider this problem more broadly, taking into account the special nonlinear quantum properties of nanostructures and changes in their properties, including under the action of laser radiation. The developed approach, along with intensity anomalies in RS layered nanostructures, explains the increase in refractive indices and the anomalous increase (~10^2 - 10^5) of the absorption of VB overtones in thin films, the maxima of the ratios of the intensities of the D/G bands in carbon materials, as well as an increase in the strength nostructure and plasticity of nanostructured media (Hall-Petch law). A key role in the concept being developed is played by resonant nonlinear-wave interactions, including for vibrational modes, which leads to strong vibrational-electronic interaction. This leads to an increase in chemical bonds and a change in electronic polarizabilities, which leads to an increase in VB in RS TMD and graphene.

1. D.Yoon, H.Moon and H.Cheong, J.of the Korean Physical Society, **2009**, v.55, № 3, 1299-1303
2. S.-L. Li, H. Miyazaki, H.Song, H. Kuramochi et. al., ACS Nano, **2012**, 6 7381-7388.

SPECTROSCOPIC STUDY OF ELECTRONIC INTERACTIONS IN "NANOCRYSTAL-MOLECULE" SYSTEMS

V. Dzhagan[a,b], O. Selyshchev[c], O. Isaeva[a], N. Mazur[a], O. Raievska[c,e], O. Stroyuk[d,e],

D.R.T. Zahn[c]

[a] *V. Lashkaryov Institute of Semiconductors Physics, Nat. Acad. of Science of Ukraine, 03028 Kyiv, Ukraine*
[b] *Taras Shevchenko National University of Kyiv, Department of Physics, 01601 Kyiv, Ukraine*
[c] *Chemnitz University of Technology, Semiconductor Physics, D-09107 Chemnitz, Germany*
[d] *Forschungszentrum Jülich GmbH, Helmholtz-Institut Erlangen Nürnberg für Erneuerbare Energien (HI ERN), 91058 Erlangen, Germany.*
[e] *Institute of Physical Chemistry, Nat. Acad. of Science of Ukraine, 03028 Kyiv, Ukraine.*

e-mail: dzhagan@isp.kiev.ua

Colloidal semiconductor nanocrystals (NCs) are currently in the focus of a sustainably growing direction of fascinating fundamental research with numerous promising applications. Along with well-developed II-VI NCs, a series of I-III-VI NC compounds have emerged in recent years as a viable alternative for light-emitting, bio-medical, and energy conversion applications[1,2]. A significant role in the properties of NCs is played by the molecules attached to their surface, which stabilize the NCs in colloids and functionalize NCs for particular applications. Tuning the NC properties by the attached molecules is one of the major research directions in the field.

In this work, by means of resonant Raman, Fourier-transform infrared, and X-ray photoelectron spectroscopies as well as optical absorption and photoluminescence (PL) we investigated the effect of charge transfer in several kinds of II-VI and I-III-VI NCs coupled to a strong electron acceptor - methyl viologen (4,4$^{/}$-dimethyl bipyridyl bication, MV^{2+}). Quenching of the NCs PL is typically used as a straightforward measure of the photoinduced charge transfer from the NC to surface-bound MV^{2+}. Directly monitoring/confirming the charge transfer on the side of MV^{2+} is more challenging. Even though, the $MV^{+\bullet}$ radical and MV^0 are colored, they are highly unstable in air oxygen and are easily oxidized back to the colorless MV^{2+}. This limits the detection of the reduced methyl viologen forms to anaerobic conditions or requires ultrafast *in situ* methods such as pump-probe transient absorption spectroscopy. Here, we implemented Raman spectroscopy as an efficient tool for *in situ* monitoring of the methyl viologen reduction by photo-excited NCs. The substantially different vibrational Raman modes of MV^{2+} and $MV^{+\bullet}/MV^0$ are used for an unambiguous distinction between the species.

Moreover, taking the advantage of quenched NC PL due to charge transfer to MV^{2+}, the phonon Raman spectra of Ag-In-S and Ag-In-S/ZnS were recorded. They allowed additional information on the NC structure to be derived, which are not accessible by X-ray diffraction or electron microscopy.

[1] O. Stroyuk, A. Raevskaya, N. Gaponik. *Chem. Soc. Rev.* **2018,** 47, 5354-5422.
[2] M.A. Boles, D. Ling, T. Hyeon, D.V. Talapin. *Nature Materials* **2016,** 15, 141–153.

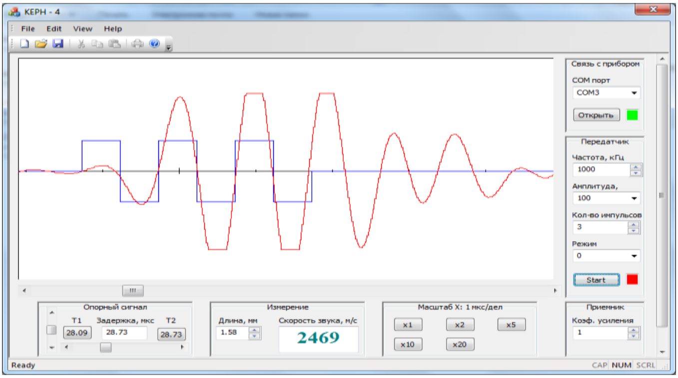
PECULIARITY OF IONEXCHANGE, ABSORBING PROPERTIES OF NANOCOMPOSITES MULTIWALLED CARBON NANOTUBES AND POLYETHYLENE, POLYVINYL CHLORIDE, POROUS POLYSTYRENE, SiO_2

A.P. Onanko, M.P. Kulish, Y.A. Onanko, D.V. Charnyi, O.P. Dmytrenko, T.M. Pinchuk-Rugal, M.A. Aleksandrov, O.L. Pavlenko, T.O. Busko, P.P. Ilyin, L.I. Kurochka
Taras Shevchenko Kyiv national university, Volodymyrs’ka str., 64, Kyiv 01601, Ukraine
e-mail: onanko@i.ua

If the dislocation segment $\xi(x,y)$, that are vibrated under the act of tension τ, is charged, additional forces will operate on it $\mathbf{F_E} = e\rho(\xi)\mathbf{E}$ and $\mathbf{F_M} = e\rho(\xi)[\frac{\partial\xi}{\partial t}, \mathbf{B}]$, where $\rho(\xi)$ - is the distribution function of electrical charge density on the dislocation segment. The system of equations, which describes the movement of the charged dislocation under act of the mechanical, electrical and magnetic fields, was transformed in to the following kind [1]:

$$M\frac{\partial^2\xi}{\partial t^2} = V_d\frac{\partial^2\xi}{\partial x^2} - Q\frac{\partial\xi}{\partial t} + b\tau - b\tau_a - N_j\frac{\partial U}{\partial\xi} + e\rho(\xi)\mathbf{E} + e\rho(\xi)[\frac{\partial\xi}{\partial t}, \mathbf{B}], \qquad (1)$$

$$\frac{\partial^2\tau}{\partial y^2} - \frac{\rho}{G}\frac{\partial^2\tau}{\partial t^2} = \rho b\frac{\partial^2}{\partial t^2}\left(\int_0^\infty [\int_0^l \xi(x)\,dx]N(l)dl\right). \qquad (2)$$



COM порт: COM3

Частота, кГц: 1000

Амплитуда,: 100

Кол-во импульсов: 3

Режим: 0

Коэф. усиления: 1

T1: 28.09

Задержка, мкс: 28.73

T2: 28.73

Длина, мм: 1.58

Скорость звука, м/с: 2469

Масштаб X: 1 мкс/дел

Figure. 1. The window illustration of data treatment of quasilongitudinal elastic waves velocity measuring $V_\parallel$ = 2469 ± 10 m/sec in the nanocomposite polyethylene with low density high pressure $(C_2H_4)_n$ + 0,7% multiwalled carbon nanotubes by impulse-phase method at frequency $f_\parallel \approx 1$ MGz.

Conclusion

1. Will consider SiO_2, GeSi crystals, which are under the combined influence of the periodic mechanical tension $\tau = \tau_0 \cdot \exp(i\omega_0 t)$, the external electric field **E** and external magnetic field **B**.

References

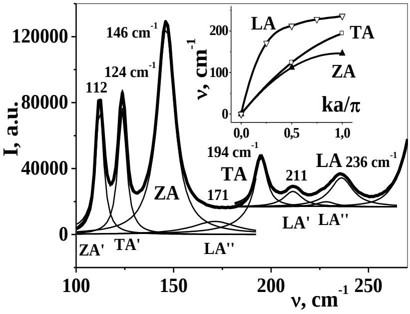
[2] O.L. Pavlenko, O.P. Dmytrenko, A.P. Onanko et al., *(PAST) Problems of atomic science and technology, series thermonuclear fusion*, **2019**, № 5(123), 94-99.

RESONANCE LASER INDUCTION OF THE ELECTRON DENSITY WAVES AND OBSERVATION OF ACOUSTIC MODES IN THE RAMAN SPECTRA OF NANO AND MICROCRYSTALLITES OF MoS$_2$

Kornienko N.E., Naumenko A.P.
Taras Shevchenko National University of Kyiv, 64/13 Volodymyrska Str., 01601 Kyiv,Ukraine
e-mail: nikkorn@univ.kiev.ua

It was previously established that the superconductivity of layered MoS$_2$ (TCR = 5–7 K) is associated with a softening of the frequencies of acoustic modes (AM) and the appearance of electron density waves (EDW). AM are not directly observed in the Raman spectra (RS) and are currently poorly studied. For MoS$_2$ nanoparticles, a decrease in the frequencies $\nu_{1,2,3}$ is shown in comparison with macro-samples: ν_1 (E_{1g}) = 287 → 279 cm^{-1}, ν_2 (E_{2g}) = 383 → 377 cm^{-1}, ν_3 (A_{1g}) = 409 → 402 cm^{-1}. With resonant excitation of RS in MoS$_2$ single crystals (λ_L = 632.8 nm), difference and sum tones $\nu_i \pm$ LA (i = 1,2,3) are observed with the participation of longitudinal AM LA. From the frequencies $\nu_i \pm$ LA, it is easy to find the frequencies LA (M) = 232 cm^{-1} and νi (M) at the boundary of the Brillouin zone (BZ) at point M. Moreover, the intensity of the allowed overtone band 2LA≈463 cm^{-1} is more than 5 times exceeds the ν_3 (A_{1g}) band, while upon excitation at 488 nm, the 2LA band is almost 20 times weaker than the intense of ν_3 (A_{1g}) band. This characterizes the increasing role of AM in MoS$_2$ single crystals under laser excitation at 632.8 nm that is resonant with A and B excitons.

We found an even more radical effect of 632.8 nm excitation on nano- (4x (20-40) nm) and microcrystallites (~ 0.2 μm) of MoS$_2$. As a result of the formation of commensurate superlattices with doubling size of unit cells (UC) and the process of addition of phonon dispersion branches, we firstly observed LA bands in RS of MoS$_2$, as well as transverse TA and torsion ZA AM bands, which is illustrated in Fig. below. Thus, as a result of laser irradiation, the vibrational states at the boundary of the BZ (point M) are transformed to the BZ center (point Γ) and are directly observed in RS. In this case, the AM frequencies are: LA = 236 cm^{-1}, TA = 194 cm^{-1} and ZA = 146 cm^{-1}, and their sequence corresponds to the arrangement of these modes in graphene. According to Fig., the maximum intensity has the torsion mode ZA. The observation of additional spectral components ZA'= 112 cm^{-1}, TA' = 124 cm^{-1} and LA' = 211 cm^{-1} (see Fig.) is due to the doubling of UC sizes. The appearance of weak additional LA″ components at 171 and 229 cm^{-1} indicates the third consecutive doubling of UC sizes. Thus, an increase in the size of UC MoS$_2$ by no less than 8 times is shown. All observed AM lines are well approximated by Lorentzians, which indicates the absence of inhomogeneous broadening. According to the repeating scenario of complication of the 2H-MoS$_2$ superstructure under the influence of resonant laser radiation of 632.8 nm, the phonon dispersion of AM was restored, as shown in the inset in Fig. In the presence of an admixture of carbon atoms, radiation of 632.8 nm leads to the appearance of CDWs in MoS2 single crystals and the observation of intense lines LA = 237 cm^{-1}, TA = 189 cm^{-1} and ZA = 151 cm^{-1}.



METABOLIC ELECTRON TRANSFER BY FRAGMENTS OF DNA MOLECULE TAKING INTO ACCOUNT THE REAL STRUCTURE OF NUCLEOTIDES

A. D. Suprun, L. V. Shmeleva
Faculty of Physics, Taras Shevchenko National University of Kyiv, 64/13,
Volodymyrska Street, Kyiv, Ukraine, 01601
e-mail: lshmel@univ.kiev.ua

Theoretical analysis of a fragment of a DNA molecule as one of the channels of metabolic electron transfer is carried out in research. The consideration is based on the experimentally established fact [1] about the real existence of such a transfer.

DNA is considered in a model of a one-dimensional molecular crystal with a mixed type of intermolecular bonds. Each elementary cell of such a crystal consists of a complementary nucleotide pair. And each such pair has two translation-invariant molecular groups (sugar phosphate backbones) and two non-translation-invariant groups (nitrogenous bases: adenine, thymine, cytosine and guanine).

The heterogeneity of each of the complementary chains is effectively taken into account. The working functional was used to find current states, electron velocity and current in nucleic acids. In it, the heterogeneity of the nucleotide chains is taken into account in the form of an averaged residual electrostatic field. Such a field arises due to heterogeneity of the nitrogenous bases. It is not equal for each of the polynucleotide chains, and is also different from the residual field between the chains. These fields induce directed electron transfer in the absence of a real external field.

The eigenvalues of the problem under consideration were found. For conduction states, they have view of four dispersion bands grouped in two pairs. In the case where the difference between polynucleotide chains is not taken into account, such structuring is absent.

Estimates were made for the current generated by an electron injected into a fragment of a DNA molecule. According to these estimates, the current decreases with increasing length of this fragment. In particular, for DNA fragments with a length of ~ 30 nucleotide pairs, the estimates for the current give a value of ~ 1.6 microamperes. And for fragments with a length of ~ 300 nucleotide pairs, the current is already ~ 16 nanoamperes. That is, an increase in the chain length by 1 order leads to a decrease in current by 2 orders. This distinguishes the conductivity of DNA from ordinary conductors or semiconductors, in which the dependence is linear.

1. Astakhova T. Yu., Likhachev V. N., Vinogradov G. A. Long-range charge transfer in biopolymers. Russian Chemical Review. 2012. **81** (11), 994-1010. https://www.turpion.org/php/paper.phtml?journal_id=rc&paper_id=4308

SYNTHESIS, MORPHOLOGY AND INTRAMOLECULAR STRUCTURE OF POLYETHYLENE GLYCOL WITH METHYLENE BLUE DYE FILMS

M.A. Alieksandrov [a], T.M. Pinchuk-Rugal, A.M. Gaponov, O.P. Dmytrenko,
A.P. Onanko, M.P. Kulish
[a] *Kyiv National Taras Shevchenko University, 01033 Kyiv, Ukraine*
e-mail: mrmarafon@gmail.com

In the last few decades, composites and nanocomposite materials have attracted worldwide attention in various fields, especially in materials science. One of the most important types is organic polymers based on inorganic materials, especially nanosize. This type of nanocomposite materials should have good properties in various applications, especially in industry.

Polyethylene glycol (PEG) is one of the most important polymers because it exhibits interesting behavior and properties, is a commercial, non-toxic, non-toxic and non-corrosive polymer.

Modification of the polymeric matrix of PEG with π-coupled systems, dyes, fullerenes C60 certainly affects the intrinsic molecular structure and properties of polymer composites. However, the structure of the polymeric matrix of PEG, its modification by different π-coupled systems has not been investigated.

Composites of polyethylene glycol films with methylene blue dye (MB) and fullerenes C60 were studied. The films of pure PEG and its composites with MB and C60 were synthesized by the «Doctor blade coating method». The morphology, crystalline structure, optical absorption of composite films were studied.

It is shown that with increasing concentration of modifiers the intramolecular structure of the composites changes, which is manifested by the shifts of optical absorption bands and in the appearance of new lines. This indicates the presence of interaction in the composites between the macromolecules of the polymer and the filler (dye), or the formation of complexes with charge transfer in the case of fullerene.

SYNTHESIS AND PROPERTIES OF NANOSTRUCTURED COMPOSITE Ce:GdAG/Cr:Al_2O_3

I.V. Berezovskaya [a], O.V. Khomenko [a], N.I. Poletaev [b], M.E. Khlebnikova [b], V.P. Dotsenko [a],

[a] A.V. Bogatsky Physico-Chemical Institute, National Academy of Sciences of Ukraine,
Lustdorfskaya doroga 86, 65080 Odessa, Ukraine;
[b]Institute of Combustion and Advanced Technologies, Mechnikov Odessa National
University, Dvoryanskaya 2, 65082 Odessa, Ukraine
e-mail: ssclab@ukr.net

Gadolinium aluminum garnet $Gd_3Al_5O_{12}$ (GdAG) doped with Ce^{3+} ions is known as the effective phosphor for white light-emitting diodes (LED,s) [1]. Also, the development of nanocomposites based on GdAG:Ce^{3+} for imaging and photodynamic therapy of cancer cells has been recently reported [2]. In this report, we discussed the synthesis and luminescent properties of nanostructured composite Ce:GdAG/Cr:Al_2O_3.

Gadolinium aluminum garnet doped with Ce^{3+} ions has been prepared by the co-precipitation of gadolinium and aluminum hydroxides and their further thermal decomposition. Cr^{3+}-doped Al_2O_3 nanoparticles with sizes of 10-70 nm were obtained by gas-disperse synthesis. The components (Ce:GdAG/Cr:Al_2O_3 ratio 2:1) were then mixed thoroughly in ethanol and after drying annealed at 1200°C in a reducing medium.

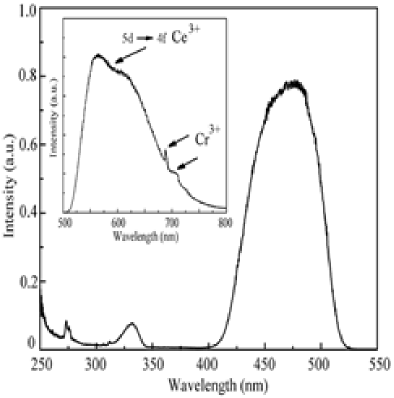


Fig. 1 Emission and excitation spectra of composite Ce:GdAG/Cr:Al_2O_3 at 77 K.

It is shown that the alumina matrix forms a barrier between GdAG:Ce^{3+} grains and suppress aggregation, grain growth of GdAG particles. Upon excitation with blue LED light the luminescent properties of the composite obtained are mainly determined by the 5d→4f transitions of Ce^{3+} in GdAG (Fig. 1), although a weak emission of Cr^{3+} from ^2E_g state in α-Al_2O_3 is also observed due to energy transfer from Ce^{3+}. Taking into account a high quantum yield of the composite (η = ~0.60 at 293 K) upon excitation at 450-470 nm it is considered as an efficient color converter for solid state lighting.

[1] Dotsenko V.P., Berezovskaya I.V., Voloshinovskii A.S. et. al., *Mater. Res. Bull.,* **2015**, 64, 151-155.

[2] Jain A., Koyani R., Muñoz C. et. al., *J. Colloid Interface Science*, **2018**, 526, 220-229.

SOLVENT EFFECTS ON PHOTOPHYSICAL PROPERTIES OF ORGANIC DYES IN THE POLYMER MATRIX

T.V. Bezrodna[a], O.I. Antonenko[b], L.F. Kosyanchuk[b], O.O. Brovko[b],
V.I. Bezrodnyi[a], A.M. Negriyko[a]
[a] *Institute of Physics NASU, 46 Nauki av., Kyiv 03680, Ukraine*
[b]*Institute of Macromolecular Chemistry NASU, 48 Kharkivske av., Kyiv 02160, Ukraine*
e-mail: tomaalone@yahoo.com

Development of efficient dye-doped solid-state laser elements requires homogeneous distribution of dopants in the solid matrices and prevention for the dye molecules to form different aggregates due to hydrogen bonds, Van-der-Waals or other interactions. The most commonly used method for the dye inclusion into the polymer matrices is incorporation to the polymer material preliminary prepared subsidiary dye solutions and subsequent solvent removal by means of vacuumization. According to the literature data, the choice of the specific solvent is arbitrary, and the main task is its removal from the mixture before the polymerization reactions. The volatile solvents are usually applied for this purpose.

This study is dedicated to the effects of the five solvents (ethylacetate, dichloromethane, acetone, ethanol, acetonitrile), different by physical parameters, on the molecule association and spectral properties of the organic dyes, doped into the polymer matrix. The organic compounds, such as, Rhodamine 6G (R6G) and Rhodamine B (RB), generated efficiently spontaneous and stimulated emission in liquid and solid-state solutions, have been chosen as laser dyes. The polymer matrix from a class of heterochain polymers, namely, polyurethane, has been used in our investigations. This material is produced by the photopolymerization reaction of oligo-urethane acrylate with a use of benzoin isobutyl ester photoinitiator, which forms radicals under ultra-violet light irradiation.

The analysis of absorption spectral curves for the dye polymer solutions allows to select absorption maxima, which relative intensity depends strongly on a type of the solvent used. Since absorption peak positions for the R6G dye are located in the 532–535 nm (monomers) and 515–518 nm (dimers) spectral regions, and these ranges for the RB dye are 555–558 nm and 532–535 nm, correspondingly, the spectral contours and maxima parameters can give information about association states of the studied dye molecules in the polymer medium.

The graphical separation of absorption spectral contours allows to select at least two spectral components in the mentioned regions and to estimate their relative intensity ratio in all dye-doped polymer samples. The monotonic increase of the absorption cross-section ratio for the dye monomer/dimer forms is observed at the growth of solvent dielectrical permittivity. The growth of solvent polarity causes intensification of the dye luminescence emission and increases the bathochromic shift. The work discusses also the effects of solvent donor-acceptor properties on the spectral characteristics of the studied dyes.

ABSORPTION OF LASER RADIATION BY METALLIC NANOPARTICLES EMBEDED IN A DIELECTRIC MATRIX IN THE CONDITIONS OF SURFACE PLASMON RESONANCE

A.A. Biliuk, O.Yu. Semchuk, O.O. Havryliuk
Chuiko Institute of Surface Chemistry of National Academy of Sciences of Ukraine, 17 General Naumov Str., Kyiv, 03164, Ukraine
s-mail: philosoph.tb@gmail.com

In recent years, increased interest in the study of optical properties of metallic nanostructures. This interest is primarily related to the practical application of such nanostructures in quantum optical computers, micro- and nanosensors [1]. These applications are based on a fundamental optical effect - the excitation of surface plasmons. Surface plasmons are electromagnetic excitations of an electron plasma of metals at the metal-dielectric interface, which are accompanied by fluctuations in the surface charge density. The consequence of this phenomenon is the surface plasmon resonance (SPR) - increase energy absorption metal nanoparticles when approaching the frequency of the incident light (laser) to the frequency SPR nanoparticles. The SPR frequency for metallic nanoparticles contained in a dielectric matrix is found in the paper. It is shown that in metal nanoparticles, oscillations of the width of the SPR line can be observed with a change in the dielectric constant of the medium in which they are. We found that both the amplitude and period of oscillations width SPR grow in small spherical nanoparticles placed in a dielectric matrix with dielectric constants greater value ε_m. However, the amplitude of plasmonic oscillations decreases quadratically with increasing radius of the spherical nanoparticle with increasing magnitude ε_m. The width of the SPR line gradually increases and increases around its smooth part Γ_0^{res}. Oscillating additive to the SPR line width $\Gamma_{osc}^{res}(R,\varepsilon_m)$ is an important amendment to Γ_0^{res}, especially for small radius particles (the SPR line oscillations are well expressed for *K* and *Ag* nanoparticles of small radii and virtually disappear for large radii nanoparticles). As the radius of the spherical nanoparticle R grows, the width of the SPR line decreases substantially and increases around a certain constant value in mediums of greater value ε_m. The magnitude of these oscillations is larger the smaller the size of the nanoparticle and increases significantly with increasing ε_m. The least acceptable radius of nanoparticles, which can be regarded as part of the reduced theory is limited to a certain value $R_{min} \simeq 0.855$ nm.

[1] Maier S. A. Plasmonics: Fundamentals and Applications.— NY: Springer, New York.- 2007.

pH-SENSITIVE PHOTOLUMINESCENCE OF $AgInS_2/ZnS$ QUANTUM DOTS IN BUFFER SOLUTIONS

L. Borkovska[a], A. Rachkov[b], J.-L. Doualan[c]
[a] *V. Lashkaryov Institute of Semiconductor Physics of NASU, 45 Pr. Nauky, Kyiv, Ukraine*
e-mail: l_borkovska@ukr.net
[b] *Institute of Molecular Biology and Genetics of NASU, 150 Zabolotnogo Str., Kyiv, Ukraine*
[c] *CIMAP, CEA-CNRS-ENSICAEN, Normandie Université, 6 Blvd Maréchal Juin,Caen,France*

The interest to luminescent colloidal semiconductor nanocrystals, quantum dots (QDs), is highly motivated by their potential application in opto- and photoelectronics, biology, medicine, etc. The $AgInS_2$ QDs show high photoluminescence (PL) quantum yield and comprise of low-toxic elements that is especially important for the *in vivo* bio-imaging.

In this work, the results of investigations of optical properties of water-soluble $AgInS_2/ZnS$ core-shell QDs in buffer solutions of different pH (3.0-9.0) are presented. The QDs were synthesized in aqueous media in the presence of mercaptoacetic acid (MAA) or glutathione.

In the PL spectra of the QDs (Fig.1), a wide PL band ascribed to carrier recombination via the levels of intrinsic defects was observed. For MAA-capped QDs it was peaked at ~633 nm and showed the Stokes shift of ~0.85 eV, while those of glutathione-capped QDs were ~587 nm and ~0.7 eV, respectively. The QDs of both types demonstrated PL relaxation dependent on the detection wavelength apparently due to variation of QDs in size.

In neutral and acidic buffers, the PL intensity increased with increasing pH from 4.0 to 7.2. Simultaneously, the PL band shifted to shorter wavelengths. The changes were more pronounced for glutathione-capped QDs. The increase of pH from 7.2 to 9.0 produced both the increase (glutathione-capped QDs) and the decrease (MAA-capped QDs) of PL intensity. These transformations of the PL spectra were accompanied by the changes of the PL relaxation times, which became longer with PL increase and shorter with PL decrease.

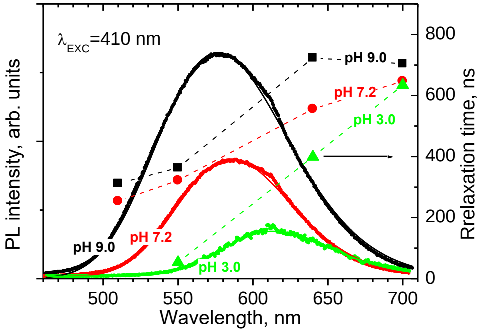


Fig.1. PL spectra and PL relaxation times of glutathione-capped QDs in buffers.

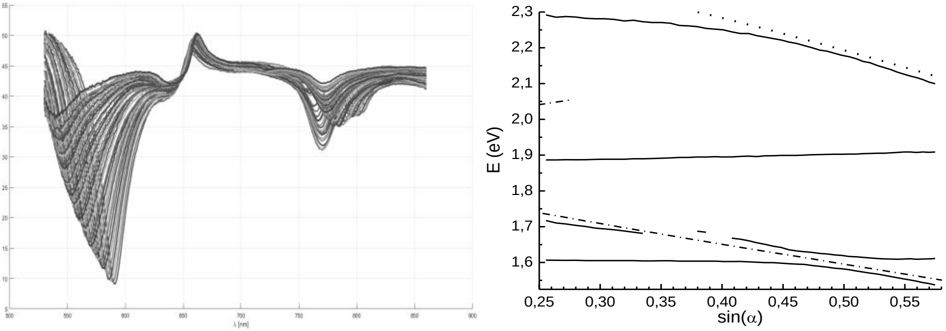
In the acidic buffer with pH 3.0, the PL intensity decreased by several times, the PL band shifted to longer wavelengths by 35 nm, and the PL relaxation times shortened. These changes were ascribed to dissociation of ligands from the ZnS outer shell, resulting in aggregation of QDs and loss of their solubility. It is proposed that glutathione-capped $AgInS_2/ZnS$ QDs may be used as a new type of fluorescence pH-sensor or indicator.

MICROELLIPSOMETRIC INVESTIGATIONS OF MIM STRUCTURES WITH ORDERED LATTICES OF PLASMONIC NANOPARTICLES

E. Bortchagovsky [a], F. Dai [b], J. Tang [b], M. Fleischer [b], I. Milekhin [c], D. Zahn [c], R. Kenaz [d], R. Rapaport [c]
[a] *V. Lashkarev Institute of Semiconductor Physics of NAS of Ukraine, pr.Nauki 41, Kyiv 03028, Ukraine*
[b] *Institute of Applied Physics, Eberhard Karls Universität Tübingen, Auf der Morgenstelle 10, D-72076 Tübingen, Germany*
c Institut für Physik, Technische Universität Chemnitz, Reichenhainer Straße 70, D-09126 Chemnitz, Germany
[d] *The Racah Institute of Physics, The Hebrew University Jerusalem, Edmond J. Safra Campus, Jerusalem 91904, Israel*
e-mail: bortch@yahoo.com

Metal-insulator-metal (MIM) structures with ordered lattice of plasmonic nanoparticles as one metallic layer have reach number of tunable plasmonic excitations interacting with external radiation and between themself. Many parameters of such a systems – geometrical sizes of nanoparticles, pitch of the lattice, the thickness of the separating dielectric, etc. govern the spectrum and hybridisation of plasmonic excitation of such a systems. Structures with gold disks of 50nm thick with variable diameter and the pitch of square lattice on glass substrate covered 50nm thick gold film separated by 11nm of SiO_2 from nanoparticles were investigated by spectroscopic microellipsometer with few microns spatial resolution.

Spectral behavior of Ψ for the angles of incidence 15^0-35^0 measured for square lattice with the pitch of about 350nm of gold disks with the diameter of about 220nm are shown in the first panel of the figure. It clearly demonstrates dispersive excitation for short wavelength, localized resonance at about 1.9eV, which spectral shape hints its interaction with the gold underlayer and complex structure at longer wavelength. Corresponding to this behavior dispersion relations shown on the second panel demonstrate interaction and splitting of modes.



EXCITONS SPECTRUM IN MULTILAYER AlN/GaN NANOSTRUCTURES

Igor Boyko, Halyna Tsupryk, Yuriy Stoianov
Ternopil Ivan Puluj National Technical University, Ruska Street 56, 46001 Ternopil, Ukraine
e-mail: boyko.i.v.theory@gmail.com

Theoretical and experimental studies [1] of electronic processes occurring in multilayer resonant tunneling structures (RTS) are crucial to ensure the efficient operation of modern quantum cascade lasers and detectors of middle and near-range electromagnetic wave, based on binary GaN, AlN and ternary AlGaN nitride semiconductor alloys. Investigations of the electron flows interaction with other quasiparticles is an integral part of such studies.

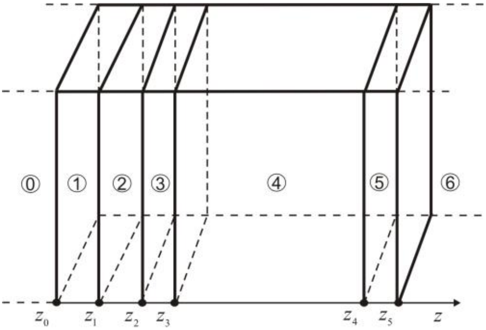


Fig. 1. Geometrical scheme of nanostructure

In proposed work, we study the spectrum of excitons arising as a result of electron – hole interaction in an AlN / GaN double-well nanostructure. The effective masses of an electron and a hole and the dielectric permittivity of a nanostructure, taking into account the notation in Fig. 1, can be represented as:

$$m^{(e,h)}(z) = m_0^{(e,h)} \sum_{p=0}^{3} \left[\theta(z - z_{2p-1}) - \theta(z - z_{2p}) \right] + m_1^{(e,h)} \sum_{p=1}^{2} \left[\theta(z - z_{2p-1}) - \theta(z - z_{2p}) \right], \tag{1}$$

$$\varepsilon(z) = \varepsilon^{(1)} \sum_{p=0}^{3} \left[\theta(z - z_{2p-1}) - \theta(z - z_{2p}) \right] + \varepsilon^{(0)} \sum_{p=1}^{2} \left[\theta(z - z_{2p-1}) - \theta(z - z_{2p}) \right] \tag{2}$$

Exciton states are determined by finding solutions of the stationary Schrödinger equation:

$$\left(-\hbar^2 \frac{\partial}{\partial z_{ex}} \left(\frac{1}{m_{ex}} \right) \frac{\partial}{\partial z_{ex}} - eFz_{ex} + U^{(e)}(z) + \Delta E_C(z_{ex}) + V_{e-h}(z_{ex}) \right) \Psi(E_n, z_{ex}) = \tag{3}$$

$$= E_{ex} \Psi(E_n, z_{ex}).$$

[1] K. Wang, T. Grange, T. Lin, et al., Broadening mechanisms and self-consistent gain calculations for GaN quantum cascade laser structures, *Appl. Phys. Lett.*.,**2018**,113, 061109.

$Pb_{1-X}Cd_XI_2$ LAYERED SEMICONDUCTOR NANOSCINTILLATOR FILMS: OPTICAL AND STRUCTURAL PROPERIES

A.P. Bukivskii[1], Yu.P. Gnatenko[1], P.M. Bukivskii[1], I.V. Fesych[2]
[1] *Institute of Physics, NASU, 46 Prospect Nauky, Kyiv 03028, Ukraine*
[2] *Taras Shevchenko National University of Kyiv, 64 Volodymyrska Str., Kyiv 01601, Ukraine*
e-mail: ap.bukivskii@gmail.com

PbI_2 layered semiconductor crystal is well known as a highly promising material applicable for developing of fast and effective cooled scintillators. In our previous works we showed that intensity of its luminescence can be significantly improved by alloying them with CdI_2 layered crystals. During the $PbCdI_2$ alloy formation PbI_2 clusters and nanoparticles are naturally formed in CdI_2 matrix which leads to the creation of several “new” stable and semi-stable energy levels and optical transitions between them. The presence of such semi-stable levels leads to photoluminescence (PL) manifestation in such crystals at the room temperature.

Lately we have been working on the development of an easy and cost-efficient method to obtain the $PbCdI_2$ alloy that would have such nanocrystalline structure and optical properties particularly high temperature photo- and X-Ray luminescence.

It was found that $PbCdI_2$ films obtained by recrystallization from the solution matches our criteria perfectly. Here we study the optical and structural properties of $PbCdI_2$ films obtained by one-step deposition method in open-air conditions. The input reagents, PbI_2 and CdI_2, were dissolved in dried N,N-dimethylformamide at room temperature. Next, this precursor solution was spin-coated on a well-cleaned silicon substrate and dried to remove the remaining solvent.

Surface morphology analysis of the obtained films performed using FEI Magellan 400 SEM microscopy setup showed that it has fairly good structural homogeneity up to 10 micrometer scale.

Optical studies, such as low temperature PL spectroscopy analysis, for the films obtained from liquid solution of different diluteness were performed using MAYA2000pro spectrometer and UTREX temperature stabilization setup. We observed that obtained materials show the same nature of the optical transitions and energy levels as the bulk crystals. PL bands of free and bound excitons, donor-acceptor pairs, autolocalized excitons and electron-and-deep-acceptor recombination are observed. The energy positions of the exciton lines at 2.490, 2.509 and 2.516 eV are associated with the formation of PbI_2 clusters of 12R, 4H and 2H crystalline modification that are formed in various film regions. It highly correlates with obtained results of X-ray dispersion analysis that showed formation of 12R, 4H and 2H polytype crystallites.

We assume that the nanoparticle growth occurs simultaneously with the crystallization of the $PbCdI_2$ solid solution (not while the solution is in liquid form) hence there is no dependence between the exciton energy and the dilution of the precursor liquid solution.

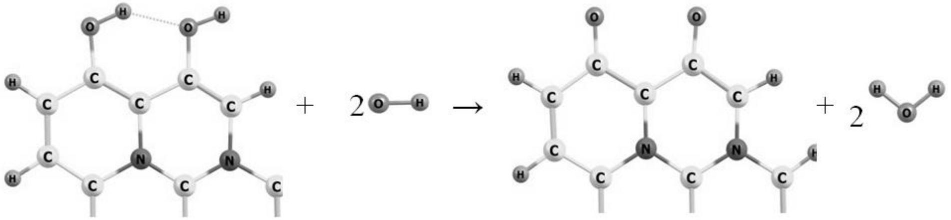
EFFECT OF NITROGEN DOPING ON THE REDOX PROCESSES ON THE SURFACE OF GRAPHEN-CLUSTERS

Demianenko E.M., Grebenyuk A.G., Lobanov V.V., Karpenko O.S., Kartel N.T.
Institute of Surface Chemistry of National Academy of Sciences of Ukraine,
17 General Naumov Str., Kyiv, 03164, Ukraine,
E-mail: Demianenko_en@ukr.net

Organic electronics have several advantages over traditional semiconductor technology. The main ones are: flexibility, low cost, transparency. The fact development of technologies, including electronic lithography, at the end of the last century, served as a basis for the formation of a new scientific direction on graphene and its derivatives, in particular, in the development of new efficient batteries, supercapacitors and fuel cells [1].

The work of these devices is based on redox reactions on the surface of graphene-like materials, their energy characteristics can be substantially improved by substituting carbon atoms by other heteroatoms, in particular, nitrogen atoms [2].

In order to determine the effect of nitrogen atoms in graphene clusters on their redox properties, the redox reactions have been examined of the transformation of hydroxyl groups into a ketone on the surface of graphene clusters of different sizes with two carbon atoms substituted by nitrogen atoms occurring according to the following scheme:



All the calculations were carried out by density functional theory method with fuctional B3LYP and basis set 6-31G(d,p) and dispersion correction by Grimme by means of Firefly 8.2.0 program package.

The calculated value of ΔG serves as a criterion for the spontaneous course of the redox reaction and allows us to find a relation between the chemical energy and the electrode potential: $\Delta G = -nFE$. It has been found that the oxidation of hydroxyl groups on nitrogen-containing carbon nanoclusters is for more than 200 kJ /mol thermodynamically plausible compared to pure carbon graphene clusters, regardless of the cluster size and the positions of the heteroatoms. The calculated electrode potentials of this reaction for nitrogen-containing and pure graphene clusters differ by more than 1.5 V.

---

[1] Bo Wang, Tingting Ruan, Yong Chen et al., *Energy Storage Materials*, **2020**, 24, 22-51.
[2] E.M.Demianenko, O.S.Karpenko, V.V.Lobanov, N.T. Kartel, *Surface*, **2017**, 9(24), 14-27.

SURFACE CENTERS OF Cr^{3+} IONS IN NANOSIZED Al_2O_3

V.P. Dotsenko[a], I.V. Berezovskaya[a], N.I. Poletaev[b], M.E. Khlebnikova[b], O.V. Khomenko[a]
and N.P. Efryushina[a]

[a] *A.V. Bogatsky Physico-Chemical Institute, National Academy of Sciences of Ukraine,*
Lustdorfskaya doroga 86, 65080 Odessa, Ukraine;
[b]*Institute of Combustion and Advanced Technologies, Mechnikov Odessa National*
University, Dvoryanskaya 2, 65082 Odessa, Ukraine;
e-mail: v.dotsenko@ukr.net

Cr^{3+}-doped Al_2O_3 samples, with particles sizes of 10-70 nm, were obtained by combustion method. The luminescence properties of Cr^{3+} ions in Al_2O_3 before and after thermostimulated phase transitions from δ^*-Al_2O_3 to θ- polymorph and then to α-Al_2O_3 have been studied and compared. It is shown that Cr^{3+} ions in as-prepared samples (δ^*-Al_2O_3) occupy octahedral sites inside and at the surface of the nanosized particles and cause several relatively narrow emission lines (R-lines luminescence) in the 680-720 nm region (Fig. 1). The local structure around Cr^{3+} ions inside the nanoparticles (regular Cr^{3+} centers) is shown to differ from that of Cr^{3+} in the surface layer, which results in essential differences in the inhomogeneous linewidth and temperature-induced shift of the R-lines. Based on the data of XRD analysis and luminescent measurements, we discuss the following aspects: - influence of impurity (Cr^{3+}) site symmetry and structural disorder on the luminescence properties; - structural disorder degree as a phase transition parameter; - nature of intrinsic defects in nanosized Al_2O_3 obtained by combustion method.

The results obtained are interpreted as a result of a) changes in distortion of the Cr^{3+} surrounding from perfect octahedral symmetry, and b) a higher degree of structural disorder in the metastable δ^*, θ-polymorphs. Because of the fine morphology and favorable particle size distribution nanosized Al_2O_3:Cr^{3+} obtained by combustion method can be of interest as an effective precursor for fabrication of transparent emitting ceramics and composite materials based on Cr^{3+}-doped Al_2O_3.

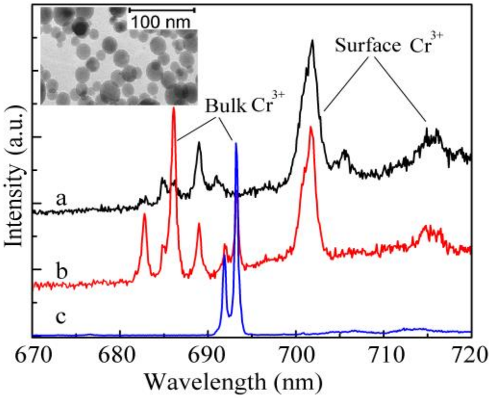


Fig 1 Influence of annealing in air on the emission spectrum of Al_2O_3:Cr^{3+} at 77 K:
(a) as-prepared sample;

(b) sample annealed at 1130°C;

(c) sample annealed at 1300°C

POSITRON SPECTROSCOPY STUDY OF DEFECTS STRUCTURE AND ELECTRONIC PROPERTIES OF POLYMER-CARBON NANOTUBE COMPOSITES

E. Tsapko, E. Len, I. Galstian, M. Rud
G.V. Kurdyumov Institute for Metal Physics of the N.A.S. of Ukraine 36 Academician Vernadsky Boulevard, UA-03142 Kyiv, Ukraine
e-mail: stenforti@ukr.net

Last year’s studies of polymer nanocomposites based on thermoplastic and thermosetting polymers (matrix) and carbon nanotubes (filler) have become widespread due to the prospects of their technical applications [1, 2]. Of particular interest are nanocomposites obtained by compacting from a mixture of dispersed polymer and filler. It provides the creation of a structural frame of filler particles in a matrix of a thermoplastic polymer, under the condition that the size of the polymer particles significantly exceeds the particle size of the filler [3, 4]. Using the method of positron spectroscopy (PS) we studied the features of the electronic structure with the determination of the characteristics of defects in nanocomposites in the concentration range from 0 to 1 wt.% of multi-walled carbon nanotubes (MWCNTs) in matrices of polyvinyl chloride (PVC) and polytetrafluoroethylene (PTFE).

It has been established that with the introduction of MWCNTs into the polymer, both in the size of defects and in the fraction of positrons that they capture are increased, compared with those in a pure polymer. However, in the entire studied range of MWCNT concentrations, these parameters remain lower than in the solid of pure MWCNTs. An analysis of the PS spectra shows that almost all positrons annihilate in MWCNTs. It means that MWCNTs are the most efficient positron capture centers in polymer-MWCNT composites even at concentrations lower than 0.1 wt.%. Higher values of the positron annihilation probability with free electrons ($P_{\theta F}$) and π-electrons (P_{rmi}) in a PVC composite with a minimum concentration (0.065 wt.%) of MWCNTs indicate the acceptor properties of MWCNTs in PVC. During the process of establishing of electrical contacts between MWCNTs, the largest changes in the annihilation parameters $P_{\theta F}$, r_{mb}, and P_{rmb} are observed, indicating an increase in the concentration of conduction electrons ($P_{\theta F}$), defect sizes (r_{mb}), and the probability of positron annihilation in them (P_{rmb}). A decrease in the positron annihilation probability with electrons in defects in the outer layer of nanotubes and the radius of localization of the electron wave function in them compared to the values of the same parameters for interlayer defects in MWCNTs points at the fact of adsorption of polymer matrix molecules on defects in the outer carbon layer of nanotubes.

[1] Z. P. Madzarevic, H. Schut, J. Cízek, and T. J. Dingemans, Free Volume in Poly(ether imide) Membranes Measured by Annihilation Lifetime Spectroscopy and Doppler Broadening of Annihilation Radiation. *Macromolecules*, 2018, **51**(23): 9925-9932.

[2] Somia Awad, Samy El-Gamal, Adel M., El Sayed Esam, E. Abdel-Hady, Characterization, optical, and nanoscale free volume properties of Na-CMC/PAM/CNT nanocomposites. *Polymers for advanced technologies*, 2020, **31**(1): 114-125.

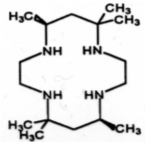
[3] Y. C. Jean, Positron annihilation spectroscopy for chemical analysis: a novel probe for microstructural analysis of polymers. *Microchem. J.*, 1990, **42**(1): 72-102.

[4] O. E. Mogensen, Positron Annihilation Chemistry. Springer−Verlag: Berlin, Germany, 1995.

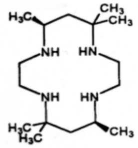
PHOTOELECTROPHYSICAL PROPERTIES OF PHOTOSENSITIVE THIN FILM STRUCTURES BASED ON HETEROLIGAND TETRAAMINE CHROMIUM(III) COMPLEXES

Gerda V.I.[a], Studzinsky S.L.[b]
[a] *Faculty of Chemistry, Departmen of Analytical Chemistry, Taras Shevchenko National University of Kyiv, 60 Volodymyrska Street, Kyiv, 01033, Ukraine.*
[b] *Faculty of Chemistry, Macromolecular Chemistry Department, Taras Shevchenko National University of Kyiv, 60 Volodymyrska Street, Kyiv, 01033, Ukraine.*
e-mail: vasyl.gerda@gmail.com

The new photosensitive thin film structures based on heteroligand tetraamine complexes of chromium (III) with halogenid-ions have been prepared. The photoelectric characteristics of these chromium (III) complexes are dependent on structure cyclic tetraamines:



meso-Me_6[14]aneN_4
(*tet a*)



rac-Me_6[14]aneN_4
(*tet b*)

and way their coordination to Cr(III).

The spectral, electrical and photoelectric properties of prepared film structures were studied. It was shown, that investigated film composites exhibit photovoltaic effect under irradiation by light from the respective chromium(III) complexes absorption region. The features of the photoelectrophysical properties of the investigated film structures, as well as the possible nature of the photovoltaic effect and charge carriers photogeneration mechanisms are discussed. The respective phenomenological model for internal photoeffect in investigated film compositions was proposed.

DONOR-ACCEPTOR INTERMOLECULAR ELECTRON BONDING AND STRUCTURAL TRANSFORMATIONS OF CHAIN-LIKE BISMUTH PENTAFLUORIDE CLUSTERS

Grebenyuk A.G.
Chuiko Institute of Surface Chemistry of National Academy of Sciences of Ukraine,
17 General Naumov Street, 03164 Kyiv, Ukraine
e-mail: grebenyuk_ag@ukr.net

Modern solid state chemistry considers the search for correlations between the structure and properties of various compounds its main task. In the case of nanoparticles, a problem arises on the effect of the surface layer on their equilibrium spatial structure and reactivity. One-dimensional (chain-like) structures can be easily investigated theoretically by quantum chemical methods within cluster approximation that involves the selection of a certain fraction of the crystal lattice, and the boundary conditions for the finite atoms must be satisfied. Since most inorganic compounds are characterized by a hypervalent structure where the coordination numbers of atoms or ions exceed their normal valences, the study of their cluster models is of particular interest.

When classifying hypervalent chain structures, they can be divided into several groups, depending on the coordination number of structure-forming atoms and the number of monatomic bridges that bind these atoms. For example, BiF_5 crystallizes in the tetragonal space group I4/m – C^5_{4h} with the shortest Bi-F distances of 1.90 (4×, side ligands) and 2.11 Å (2×, Bi-F-Bi bridges).

Due to the absence of atoms required to complete the coordination sphere of the finite atoms of clusters (which is characteristic of any hypervalent structure), sometimes their equilibrium spatial structure may be distorted or even regroup under conditions of optimization of geometry due to saturation of coordinating valences. The formation of intermolecular complexes with additional small molecules or the parallel arrangement of several oligomer chains can help to avoid such an undesirable side effect.

Various types of molecular models (simple chains, cycles and square rings as well as combined species of brush-like or sheaf-like shape) for bismuth pentafluoride involving from 2 to 40 formula units have been examined by the density functional theory method (DFT) with the exchange-correlation functional B3LYP and the valence-only basis set SBKJC. All the calculations were performed using software GAMESS (FireFly820 version, created by A. Granovsky). The results obtained lets it possible to reproduce semi-quantitatively available experimenal data on the spatial structure [1] and thermodynamic characteristics [2] of the substance and to make an assumption about the surface structure of its crystals.

[1] C. Hebecker, *Zs. anorg. allg. Chem.*, **1971**, 384(2), 111-114.

[2] J. Fischer and E. Rudzitis, *J. Am. Chem. Soc.*, 1959, 81(24), 6375-6377.

DISPERSION OF VIBRATIONAL AND ELECTRONIC STATES AND FINE SPIN-DEPENDENT STRUCTURE OF THEIR ENERGY LEVELS IN HEXAGONAL BN CRYSTALS

V. Gubanov, A. Naumenko, I. Dotsenko
Taras Shevchenko National University of Kyiv, 64/13 Volodymyrska Str., 0160, Kyiv, Ukraine
e-mail: vagubanov46@gmail.com

The dispersion dependences of vibrational modes and electron excitations in BN crystals as well as in nitrid-borene (or BN-monolayer, $(BN)_{L,1}$) have been studied taking into account the electron spin for electron excitations.

For the first time, projective classes, which transform spin-dependent electronic wave functions at the points of high symmetry of the Brillouin zones have been determined for the above-mentioned structures. For the first time we found the method of the constructing of factor systems, in particular, the correct factor systems for spinor representations.

The dispersion of the electronic states has been investigated by using the symmetric theoretical group methods. Taking into account the symmetry to inversion of time, compulsory spin-depent thin splitting of energy spectra at different points of Brillouin zones.

It is shown that the results of the developed methods of theoretical-group analyses are consistent with the data of experimental and computational studies of energy spectra and multiplicities of degeneration of quantum states.

SPECTRAL PROPERTIES OF NILE RED DYE AT THE SILICA NANOSURFACE AND LIQUID MEDIA

Khristenko I. V., Vasilieva A. V. , Ivanov V. V.
V.N. Karazin Kharkiv National University, School of Chemistry,
Svoboda sq., 4. Kharkiv, 61022, Ukraine
e-mail: khristenko@karazin.ua

Nile red dye (9-(diethylamino)-5H-benzo[a]phenoxazine-5-one, NR) is characterized by high dipole moment and quantum fluorescence yield. It lead to pronounced solvatechromic and fluorochromic properties of NR. Such spectral sensitivity of the dye to polarity of the media makes it as a popular fluorescent probe for various media (cell structures, liquid media, films, surfaces *etc*). The aim of the present work is theoretical and experimental investigation the spectral properties of NR in different media (organic solvents of different polarity, in acetonitrile in the presence of copper ions and on the surface of modified silica gel). In order to provide clear interpretation of experimental data the quantum-chemical calculations by means of time dependent density functional theory (TD-DFT) were performed.

A special question of the TD-DFT calculations was concerned to necessary choice of corresponding DFT functional, basis set, and solvatation model to adequate description of spectral characteristics. Among the different DFT functionals the standard exchange-correlation functional B3LYP as well as CAM-B3LYP, PBE0, HSE, M062x were used. The effects of equilibrium and nonequilibrium solvatation in description of spectral properties were discussed. As an example the wavelength in maximum of absorption and emission for NR dye presented in the table 1 below (6-31++G(d,p) basis set was used).

Table 1. Absorption and emission λ_{max} (nm) for NR

Media	absorption			emission		
	B3LYP	CAM-B3LYP	Experim.	B3LYP	CAM-B3LYP	Experim.
Vacuum	463	405	N/A	499	470	N/A
Cyclohexane	497	435	496	533	508	565
Acetonitrile	514	455	529	604	584	617
Ethanol	514	454	547	601	581	639

Also the spectral characteristics of NR in acetonitrile in the presence of Cu^{2+} ions have been investigated. It was found that the absorption spectrum of the dye is sensitive to Cu^{2+} ions concentration.

ELECTRONIC AND MAGNETIC PROPERTIES OF NITROGEN/IRON-DOPED GRAPHENE-LIKE HEXAGONAL NANOCLUSTERS

Karpenko O.S., Demianenko E.M., Lobanov V.V., Kartel M.T.
Chuiko Institute of Surface Chemistry of National Academy of Sciences of Ukraine,
17 General Naumov Str., Kyiv, 03164, Ukraine
e-mail: karpenkooksana@ukr.net

Graphene is a material that has found wide application in various fields of chemistry, physics and of microelectronics electronic base production. Its universality is, at least in part, due to the electronic structure of an infinite two-dimensional graphene sheet, namely, the zero density of one-electron states in the vicinity of the Fermi level. This feature in many cases reflects the scope of use of graphene, which implies its modification.

The proposed report presents the results of quantum-chemical calculations (DFT, B3LYP, 6-31G**) of equilibrium spatial structure and electronic structure of hexagonal-shaped graphene nanoclusters doped with nitrogen and iron atoms. As a base, a polyaromatic molecule (PAM) of $C_{96}H_{24}$ was selected, in which two central carbon atoms were removed to form a cluster $C_{94}H_{24}$ with double vacancy (DV). Further, two and four carbon atoms, which framing the DV, were replaced by nitrogen atoms, resulting in clusters $C_{92}N_2H_{24}$ and $C_{90}N_4H_{24}$, respectively. In the centre of clusters $C_{94}H_{24}$, $C_{92}N_2H_{24}$ and $C_{90}N_4H_{24}$ the Fe atom in the oxidation states 0, +2 and +3 was placed with DV. The energies of formation, the energies of replacing carbon atoms by nitrogen atoms, the energies of binding nitrogen and/or energies of binding iron ions, the positions of peaks maximums N(1s), Fe(1s), and Fe(3d) in the scale of the electrons energy binding were calculated for all considered systems.

The results of calculations showed that the formation of carbon vacancies in graphene is energetically unfavourable, while the reactions of replacing carbon atoms by nitrogen atoms are more favourable due to less endothermic effect. Unlike the initial $C_{96}H_{24}$ PAM, for many clusters containing N and Fe atoms, the electronic ground state is not singlet, which determines their ferromagnetism and the possibility to creating permanent magnets based on them. Hybridization of the atomic orbitals of the Fe(3d) and N(2p) atoms leads to the formation of the Fe–N covalent bond and a finite density of one-electron states at the Fermi level.

OPTICAL ABSORPTION OF POLYAMINOARENES DOPED WITH ELECTRON ACCEPTOR NANOCLUSTERS

Konopelnyk O.I.[a], Rabiy V.I., Aksimentyeva O.I.
[a] *Ivan Franko National University of Lviv,*
Dragomanova, 19, Lviv, 79005, Ukraine,
e-mail: konopel@ukr.net

A great attention now attracts the conjugated polymers with intrinsic electron conductivity such as polyaminoarenes - polyaniline (PAN) and its derivatives poly-ortho-anisidine (PoA) and poly-ortho-toluidine (PoTI) because of their interesting electro-optical properties. The main factors that change the electronic properties of these polymers – energy of band gap, concentration of charge carriers or their mobility are their doping with electron donor or electron acceptor substances that generates the charge carriers of n- or p-type [1]. We have studied the effect of doping of polyaminoarenes on their structure and optical absorption in visible and near IR spectral range. All films samples on the transparent tin oxide substrates were prepared by electrochemical polymerization method in the cyclic potential mode. As doping agents were chose the substances capable to accept the electrons from π-conjugated chain – nanoclusters of graphene oxide (GO), ferric chloride ($FeCl_3$) and complex $K_3[Fe(CN)_6]$.

According to the results of the XRD analysis the PAN, PoTI and PoA films are characterized predominantly by amorphous–crystalline structure. For PAN doped with $FeCl_3$ a group of narrow, well-formed peaks corresponding to interplanar distances d = 13.46 Å and 3.43 Å indicates the formation of the phase with high crystallinity degree. Doping of PoTI and PoA by nanoclusters saves of the amorphous structure with the diffusion maximum corresponding to interplanar distance d = 14.887 Å (PoTI) and 5.79 Å (PoA).

The polyaminoarene films are characterized by absorption band in the range of $\lambda = 380 - 420$ nm, due to π-π^* transitions in conjugated aromatic system. The second band is observed in the range of 580 − 600 nm and is associated with the n→p transitions in benzo-quinoid system of polymer chain. Absorption band with maximum at 720 nm corresponds to the absorption of delocalized charge carriers.

Doping of polyaminoarenes with nanoclusters causes the changes in films coloration that corresponds to spectral changes in the visible and NIR range. In the result of doping of PoA film with GO the calculated optical band gap decreased from 1.21 eV to 1.14 eV. An interaction of ferrum ions with macrochain of polyaminoarenes occurs by the mechanism of acceptor doping, where the ions Fe^{3+} serve as an acceptor that reduced to Fe^{2+} and can oxidate the polymer chain. These processes cause an increase of the concentration of the charge carriers, and accordingly, an increasing of the optical absorption both in polaronic and in bipolaronic bands. The formation of a complex type $[PAN]^+[FeCl_4]^-$ causes the shift of the absorption maximums at $\lambda_{max} = 380$ and 820 nm to shortwave region. In this case doping of PoTI film by $FeCl_3$ can form a charge transfer complex, which leads to an increase in the intensity of the first absorption band. Introduction of $K_3[Fe(CN)_6]$ complex to the PoTI film causes the increase an intensity of the band at 620 nm and the disappearance of absorption induced by delocalized charge carriers.

[1] O.I. Aksimentyeva, O.I. Konopelnyk, [et al.] // Chapter 3: Computational and Experimental Analysis of Functional Materials – Toronto, New Jersey: Apple Academic Press, CRC Press. **2017**. 532 p.

DYNAMICS OF ELECTRON TRANSFER IN MELANIN-TRINITROFLUORENONE SYSTEM

A.O. Kostetskyi[1*], Yu.P.Piryatinski[1], A.B.Verbitsky[1], P.M.Lutsyk[2], A.Rozhin[2]
[1]*Institute of Physics of NAS of Ukraine, Prosp.Nauki 46, Kyiv, Ukraine*
[2] *Aston University, Aston Triangle, B47ET Birmingham, UK*
e-mail: tohakostet@gmail.com

The kinetics of photoluminescence (PL) and time-resolved emission spectra (TRES) of melanin solutions with an effective electron acceptor 2,4,7-trinitrofluorenone (TNF) have been studied.

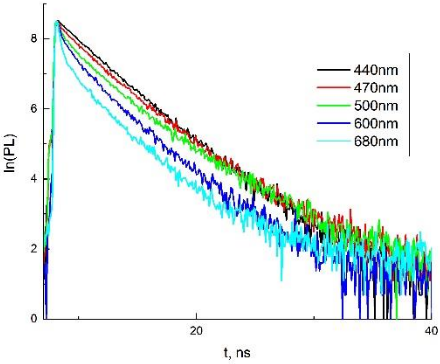
Earlier we have shown that molecules of nanostructured melanin formed two-component system with electron acceptor TNF [1] and assembled in nano-aggregates with formation of CT states [2].

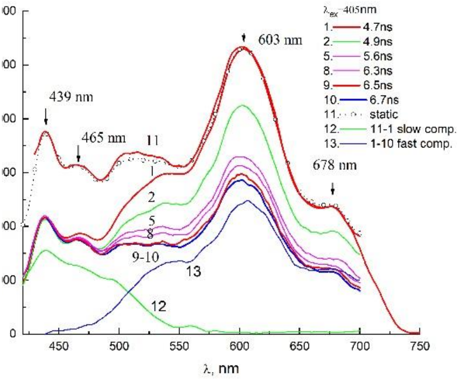
Based on the analysis of the kinetic decay curves (Figure 1), the fast and slow PL decay components can be distinguished, which characterize the processes of a relaxation of excited states and charge transfer in the melanin-TNF molecular system.

Figure 2 shows TRES spectra, characterizing the change in PL spectra in the time range up to 7 ns with the indication of fast and slow components curves.

The reasons of observed dependences are discussed and the model to explain such behavior of PL dynamic characteristics is proposed.

Fig. 1. Kinetics of PL decay for solutions of melanin-TNF system. Fig 2. TRES spectra of melanin-TNF system





[1] Verbitsky, A.B., Rozhin, A.G., Lutsyk, P.M., Piryatinski, Yu.P., Perminov, R.J. (2014). Mol. Cryst. Liq. Cryst., 589, 209.

[2] Kostetskyi A. O., Piryatinski Yu. P., Verbitsky A. B., Lutsyk P. M. & Rozhin A. G. (2018). *Mol. Cryst. Liq. Cryst*., *671:1*, 41-54.

POLYMER-POLYMER COMPOSITES BASED ON WATER-SOLUBLE POLYMERS AND POLYANILYLINE

V. Dutka, Ya. Kovalskyi, O. Aksimentyeva, T. Virsta, H. Halechko
Ivan Franko National University of Lviv, Kyryla & Mefodiya Str., 6, 79005 Lviv, Ukraine
e-mail: yaroslav.kovalskyi@lnu.edu.ua

Polymer-polymer composites (PPCs) have unique properties that make them promising for use in many electronic devices. The conductive component is polyaniline (PANI) and water-soluble polymers, such as polyvinyl alcohol (PVA), polymethacrylic acid (PMAC), and styrene copolymer with maleic anhydride (SMA), which are part of such PPCs are of great interest since along with conductivity they have film-forming properties [1, 2]. The kinetic peculiarities of PPCs formation in the process of oxidative polymerization of aniline in the presence of PVA and SMA were studied. By varying the content of the PANI in the polymer matrices, it is possible to adjust the electrical conductivity (σ) of composites over a wide range. The study of σ dependence on the temperature for the interval of T = 273-393 K allowed us to calculate the activation energy of the charge transport (E_a). Numerical values of E_a = 0.38-0.64 eV indicate that the PPCs studied are typical organic semiconductors. Besides this, the presence of a polymer matrix doesn’t change a character of the optical absorption of PANI films in the range of λ = 380–1100 nm [1].

One of the important properties of PPCs is their thermo-mechanical (TM) properties, which affect the performance and durability of devices formed with their participation. The TM curves of PVA and SMA have a classic character and the glass transition temperature determined for these polymers is consistent with the literature [2]. Studies of the thermo-mechanical properties of PPCs based on PVA and PANI and SMA and PANI indicate a strong interaction between the components. The interaction of PANI with polymer matrices was confirmed by the X-ray method and IR spectroscopic studies. The quantum-chemical calculation indicates the strong polarization of PANI molecules that can form hydrogen bonds with PVA, PMAC and SMA macromolecules. The morphological properties of the obtained polymer-polymer composites were studied.

[1] O. I. Aksimentyeva, B. R. Tsizh, Yu. Yu. Horbenko, et al. *Mol.Cryst.Liq.Cryst.*, **2018**, 670, 3–10.
[2] V. Dutka, O. Aksimentyeva, H. Halechko, Ya. Kovalskyi, *Proceedings of NTSH. Chem. Science.*, **2018**, LIII, 164–169 (in Ukr.).

IONIC CONDUCTIVITY OF GLYCOPOLYMER NETWORKS BASED ON XANTHAN AND BLOCKED POLYISOCYANATE IN THE PRESENCE OF GLICEROL

Nataly Kozak, Katerina Didenko, Zoja Gagolkina, Stanislav Nesin
Institute of Macromolecular Chemistry of the National Academy of Sciences of Ukraine,
Kharkiv chaussee, 48, Kyiv 02160, Ukraine
e-mail: kozaksmalt@ukr.net

Biopolymers are interesting renewable, biocompatible and biodegradable reagents to synthesize advanced materials with versatile technical, chemical and physical properties. Microbial exopolysaccharide xanthan (with cellulose like main chain and trisaccharide side chains consisted of β-D-mannose, β-1,4-D-glucuronic acid and β-1,2-D-mannose residues together with a pyruvic acid unit) represents anionic branched hetero-polysaccharide. Modification of the polysaccharide by blocked polyisocyanate (PIC) allows formation of cross-linked glycopolymer (GP) via interaction of hydroxyl groups of xanthan with reactive isocyanate groups that are recovered at PIC deblocking temperature.

Biodegradable polysaccharide based GP networks with calculated degree of polysaccharide hydroxyl group substitution of 20, 40, 60, 80 and 100% obtained according procedure described in [1-3] are acid-, alkali- thermo resistant and they demonstrate good ability to absorb the transition metal ions and some aromatic compounds from their water solution.

According to dielectric relaxation spectrometry measurements cross-linked GP systems in the presence of glycerol demonstrate ionic conductivity with σ_{dc} level up to 10^{-4} S/cm. Glycerol, used as GP network plasticizer, is interesting among nonaqueous solvents due to its relatively high boiling point and ability to hydrogen bonding like water. Influence of the model low molecular hydroxyl containing plasticizer on rise of macro chains mobility of GP networks was analyzed using nitroxyl spin probe. WAXS diffractograms of wet and dried GP samples show the crucial changes in short ordering in the unmodified polysaccharide whereas PIC cross-linked GP sensitivity to drying procedure diminishes with increase of modifier content in reaction mixture.

[1] N.Kozak, Yu.Nizelskii, R.Gvozdjak, S.Vocelko *9th International Conference on Chemistry of Oligomers,* Odessa, **2005**, *249*

[2] N.Kozak, Yu.Nizelskii, N.Mnich *UA Patent №85207,* **2009**,

[3] N. Kozak, A.Hubina *Current Trends in Polym Sci,* **2012**.23-27

SPECTROSCOPIC INVESTIGATION OF CHLORINE-BASED PHOTOSENSITIZERS IN POLYMER MATRIX

A. Naumenko[a], N. Kutsevol[a], V. Zorin[b]
[a]*Taras Shevchenko National University of Kyiv, 64/13 Volodymyrska Str., 01601 Kyiv,Ukraine*
[b] *Belarusian State University, 4, Nezavisimosti avenue, 220030, Minsk Republic of Belarus*
e-mail: a_naumenko@univ.kiev.ua

Photodynamic therapy (PDT) is a promising alternative treatment for cancer. To carry out this method of therapy is constantly looking for new photosensitizers (PS) - compounds that selectively accumulate in diseased cells and exhibit photo-toxicity under the action of radiation of a given wavelength. The purpose of this work was to investigate the absorption and fluorescence spectra of chlorin e6 (Ce6) and di- and trimethyl ether chlorine e6 (DME and TME, respectively) both in aqueous solutions and in the presence of branched polymers of Dextran-polyacrylamide (DPAA). The analysis of spectra show the strong dependences of spectral position and line shape of the characteristic bands from the type of polymer matrix and the photosensetizer hydrophobicity.

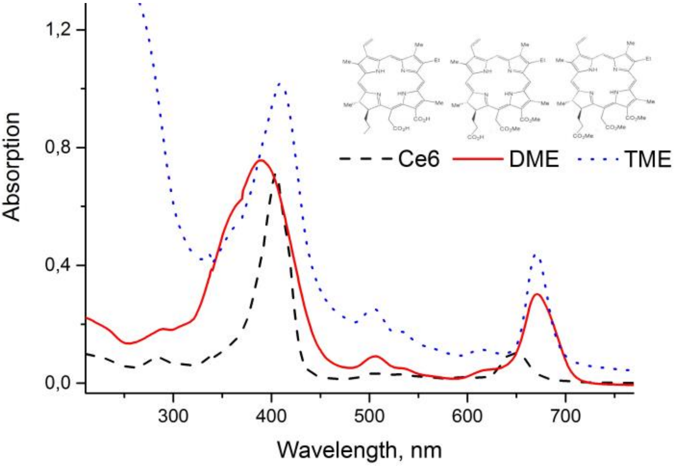


Figure 1. Changes of spectral positions of characteristic absorption bands of Chlorin e6 and its di- and tri- methyl ethers

Acknowledgements. This publication is supported in part by the Ministry of the Educationn and Science of Ukraine: joint Ukrainian-Belarussian research and development project “Design and physico-chemical properties of novel multycomponent nanosystems for the treatment and diagnostics of solid tumors” (2019-2020)

CORRELATION BETWEEN STRUCTURAL AND SPECTROSCOPIC PROPERTIES OF Sm^{3+}-DOPED $MgAl_2O_4$ NANOCRYSTALLINE SPINEL

K. Lamonova[a,*], I. Danilenko [a], O. Gorban [a], G. Volkova [a], S. Orel [a], and Yu. Pashkevich [a]
O. Viagin [b], P. Maksimchuk [b], V. Seminko [b], and Yu. Malyukin [b]
V. Kurnosov [c]
[a]*O. O. Galkin Donetsk Institute for Physics and Engineering NAS of Ukraine, Nauky av., Kyiv-03039, Ukraine*
[b]*Institute for Scintillation Materials NAS of Ukraine, Nauky av., Kharkiv-61072, Ukraine*
[c]*B. I. Verkin Institute for Low Temperature Physics and Engineering NAS of Ukraine, Nauky av., Kharkiv-61103, Ukraine*
[*]*e-mail: k.v.lamonova@ukr.net*

We report structural and optical properties of the nanocrystalline Sm^{3+}-doped $MgAl_2O_4$ orange-red phosphors with samarium concentrations of 0.03, 0.1, 0.2, 0.3, 0.5, 1.0, 1.5, and 3 wt.%. The reverse co-precipitation method was applied to synthesize the $MgAl_2O_4$:Sm^{3+} samples. X-ray phase analysis and transmitted electron microscopy have detected: (a) the presence of inverse $Al^{tet}(MgAl)^{oct}O_4$ phase in the normal $MgAl_2O_4$ spinel ; (b) the pure $MgAl_2O_4$ nanocrystals synthesized at 700ºC are in the amorphous state, and the smallest samarium addition induces the formation of a crystalline spinel phase; (c) the sizes of nanocrystals synthesized at 700ºC vary from 5 nm to 6 nm and from 7 nm to 15 nm at 1000ºC.

The sample synthesized at 700ºC and a samarium content of 1.5 wt.% exhibits a maximum of the integral intensity. This sample is the most promising candidates for use as orange-red emitting phosphors. The average size of the nanoparticles is about 5.5 nm. Additional annealing of the $MgAl_2O_4$:Sm^{3+} samples leads to the luminescence quenching process. There is near-surface samarium ions segregation in the nanocrystals with an average size of 10 nm and concentrations of 1.0 wt.% and 1.5 wt.%.

We propose a mechanism for the formation of the luminescence spectrum of the $MgAl_2O_4$:Sm^{3+} nanocrystals based on semi-empirical calculations of the samarium electron structure by the Modified Crystal Field Theory (MCFT) [1]. Numerical analysis of the luminescence spectra revealed that Sm^{3+} substitutes Al^{3+} both octahedral and tetrahedral positions. As a result, two types of coordination complexes like [SmO_6] and [SmO_4] occur. Both kinds of complexes are highly distorted due to the large difference between the samarium and aluminum ionic radii. The segregation process leads to the appearance of complexes with broken bonds, with non-equivalent bonds and complexes with oxygen vacancies. The calculations show that the most intense transitions arise in coordination complexes with vacancies, as well as in the tetrahedral [SmO_4] complexes due to the absence of the space inversion. The luminescence intensities from complexes that are deformed due to the location near the surface are two orders of magnitude smaller. Their presence in the nanoparticles influences the broadening of the luminescence bands.

[1] K. V. Lamonova, S. M. Orel, and Yu. G. Pashkevich, Modified crystal field theory and its applications, Kyiv: *Academperiodyca*, **2019**.

INFLUENCE OF POLYMER MORPHOLOGY AND METHOD OF COMPOSITE SYNTHESIS ON THE DIELECTRIC PROPERTIES OF NANOCARBON COMPOSITES

Lazarenko O., Syvolozhskyi O., Zhuravkov O., Matzui L.
Department of Physics, Taras Shevchenko National University of Kyiv,
64/13, Volodymyrska Street, City of Kyiv, Ukraine, 01601
e-mail: alazar@univ.kiev.ua

An important parameter of quality of composite consisted of dielectric polymer and conductive nanocarbon filler is the filler dispersion in the polymer volume. The tendency of high aspect ratio particles to agglomeration impairs the transport properties of composites the manufacture of so-called segregated composites allows the formation of an electrically conductive framework with a high local filler density and provides a uniform distribution of the filler in the volume of the composite sample. Depending on the method of manufacturing of segregated systems, there are different values of percolation transition φ_c, conductivity, the dielectric properties of CM, while φ_c does not depend on the type of polymer matrix, and determined by the ratio of the sizes of the filler and the polymer particles, as well as the shape of the filler [1].

The aim of this work is to investigate the influence of fabrication parameters and components types on the electrophysical characteristics of segregated polymer-nanocarbon structures. For this purpose, two different types of polyethylene powder were used as the polymer matrix: low-density polyethylene powder (high-pressure polyethylene) with a particle size of 0.1-0.3 mm and high molecular weight high-density polyethylene with a particle diameter of 100 μm. Graphite nanopletelets, thermally exfoliated graphite, and multiwall carbon nanotubes were used as conductive fillers. The dielectric permittivity and electromagnetic response parameters of the fabricated composites were investigated in the frequency range 40-60 GHz depending on the component types and temperature of the hot pressing of composites. It is shown that the size distribution of polymer particles and their morphology play the same prominent role in improving the dielectric properties of the composite as the type and the morphology of the carbon filler.

[1] Ye.P. Mamunya, et al., *Journal of Non-Crystalline Solids,* **2010,** Vol. 356 pp. 635–641.

PHOTOLUMINESCENCE IN GAS ENVIRONMENTS ZnO NANOPOWDERS DOPED BY In AND Ga

I.V. Lazoryk[a], Yu.I. Venhryn[a], A.S. Serednytski[a], D.I. Popovych[a,b]
[a] *Pidstryhach Institute for Applied Problems of Mechanics and Mathematics NAS of Ukraine*
Naukova str., 3b, Lviv-79060, Ukraine.
[b] *Faculty of Physics, Ivan Franko National University of Lviv*
Kyrylo and Mephodiy str. 8, 79005, Lviv, Ukraine
E-mail: popovych@iapmm.lviv.ua

Recently, development of gas sensors based on metal oxides nanostructures with high sensitivity and selectivity is of great interest for the determination of toxic, explosive and flammable gases in the environment. Zinc oxide is one of the promising materials for use as the gas sensor. The paper studied the characteristics of photoluminescence (PL) in various gas environments of ZnO nanopowders doped In and Ga at room temperature. Nanopowders were obtained and doped by the method of pulsed laser ablation [1]. PL studies of carried out on an installation using for excitation a UV LED (λ=365 nm). As the gas environment changes, additional adsorption centers of luminescence appear on the surface of the nanopowders, which explain the change in the intensity on the PL spectra [2]. Four elementary bands with peaks of about 430, 480, 515, and 550 nm were detected using the Alentsev-Fock method (fig.1), which indicates that there is a joint emission of transitions involving different defects. The doping of zinc oxide with indium and gallium has shown that the increase in radiation intensity is caused by the increase in the concentration of free carriers (the intensity changes due to excess charge). These studies show that ZnO:In and ZnO:Ga nanopowders are promising materials for gas-based sensors, since their functioning is based on the modification of properties due to the adsorption of gas molecules on the surface.

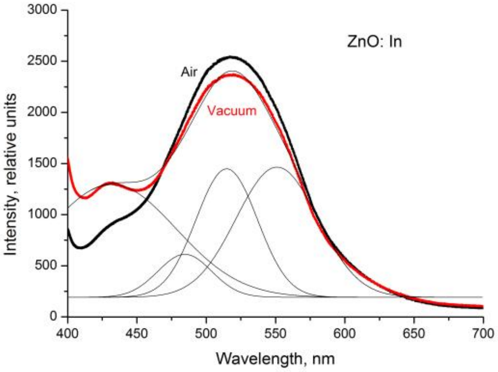


Fig.1 Decomposition of the PL spectra of ZnO:In nanopowders

1. V.V.Gafiychuk, B.K.Ostafiychuk, D.I.Popovych, I.D.Popovych, A.S.Serednytski, *Applied Surface Science*, 2011, 257(20), p.8396-8401.

2. V.M.Zhyrovetsky, D.I.Popovych, S.S.Savka, A.S.Serednytski, *Nanoscale Research Letters.*, 2017, 12, 132(5).

EFFECT OF ELECTRON SCATTERING BY IMPURITY ON THE ELECTRONIC STRUCTURE, TYPE AND SPATIAL CHARACTERISTICS OF NANOSCALE REGIONS OF MAGNETIC ORDERING IN ALLOYS

E. G. Len[1,2], V. V. Lizunov[1], T. D. Shatnii[1], M. V. Ushakov[1], T. S. Len[3]
[1]G. V. Kurdyumov Institute for Metal Physics of the N.A.S. of Ukraine,
36 Academician Vernadsky Boulevard, UA-03142 Kyiv, Ukraine
[2]Kyiv Academic University, NAS and MES of Ukraine,
36 Academician Vernadsky Blvd., UA-03142 Kyiv, Ukraine
[3]National Aviation University, 1 Kosmonavt Komarov Ave., 03058 Kyiv, Ukraine
e-mail: len@imp.kiev.ua

The description of electronic processes in systems with strong electron-electron correlations remains a complex and not yet finally solved problem because of the same order of magnitude of the interaction energy between electrons and their kinetic energy. An existence of strong correlations in electrons motion determines the unique physical properties of strongly correlated systems (SCS). There are two major problems in the theory of such systems, namely, the correlations in the SCS are often nonlocal in time and in space. Nowadays, the first problem is chiefly solved within the method of dynamical mean-field theory. The second problem is mainly decided by cluster methods. In the present work, we consider the case of absolute zero of temperature, which makes it possible to use a static approximation, and we use the cluster method to describe the spatial nonlocality of correlations. This approach is convenient because it can be extended to magnetic alloys with strong electron correlations and with arbitrary degrees of short and long atomic and magnetic orders [1]. As determined, the correlations in orientation of localized magnetic moments at nearest sites of a crystal lattice has more complicated influence on the energy spectrum of electrons in magnetic binary substitution alloys in comparison with one-component magnetic systems. In magnetic alloys, the maximal antiferromagnetic order does not lead to the obligative appearance of a full gap in total density of electronic states, but, as a rule, a quasi-gap with non-zero total density appears due to the overlapping of different impurity bands with a possible own full gap. The electron scattering processes on clusters of two or more lattice sites form peculiarities on the density of states associated with maximal magnitudes of correlations in the orientation of magnetic moments at nearest sites, which provide the largest length of homogeneous magnetic ordering regions. Impurity scattering processes lead to redistribution of charge and spin densities between atoms of different types. For example, at equal concentrations of binary alloy components, it provides bigger values of localized magnetic moments on screened ions with smaller values of potential energy of electrons. Different magnetic moments on ions of different types, in turn, lead to different splitting of impurity bands into Hubbard subzones due to the Coulomb potential (U) of repulsion of electrons at one lattice site, and to breaking of both the symmetry of the electronic density of states of the magnetic alloys relative to the centre of energy band and the symmetry of the 3D magnetic phase diagram in the variables U-n-P^{A} with respect to both half-filling of band (n = 1) and equal concentration of binary alloy components ($P^{\mathrm{A}} = P^{\mathrm{B}} = 0.5$). A difference in the concentrations ($P^{\mathrm{A,B}}$) of the alloy components (A, B) is an another essential cause of the violation of such symmetries.

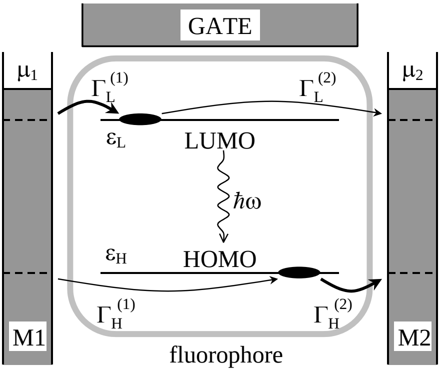
[1] E. G. Len, V. V. Lizunov, T. S. Len, M. V. Ushakov, V. A. Tatarenko, *Metallofiz. Noveishie Tekhnol.*, **2015**, 37, 1405–1424.

THE INFLUENCE OF GATE POTENTIAL ON THE FORMATION OF ELECTROLUMINESCENCE IN A MOLECULAR PHOTODIODE

V.O. Leonov, Ye.V. Shevchenko, E.G. Petrov
Bogolyubov Institute for Theoretical Physics, Metrolohichna str. 14-b, Kiev, 03680, Ukraine
e-mail: leogluck@gmail.com

Molecular photodiode is a nanoscale structure consisting of a fluorophore that is placed between two metal electrodes (1M2-system). Under certain conditions, the energy of electrons transported through such a system can be converted to the energy of quantum of light. Essentially this process is the same that occurs in organic LEDs. The difference is that the radiation of the molecule-fluorophore occurs in the nanoscale space, which, due to the formation of plasmons, enhances the radiation. Another important difference is that the efficiency of fluorophore electroluminescence highly depends on the kinetics of transitions between the states of a molecule in its charge-neutral (ground and excited) states and states with excess or deficient electron.

The figure shows the scheme of formation of electroluminescence at positive polarity bias applied to the electrodes M1 and M2, voltage bias $V = (\mu_1 - \mu_2)/|e|$ (μ_1, μ_2 are chemical potentials, $|e|$ is the electron’s absolute charge) under conditions where the electron jump rate $\Gamma_L^{(1)}$ from M1 to the LUMO exceeds the rate $\Gamma_L^{(2)}$ of the transition from LUMO to the unoccupied M2 level. In addition, in the same asymmetric photochromic molecule, the rate $\Gamma_H^{(2)}$ of the electron transition from a double-populated HOMO to M2 is believed to exceed the rate of $\Gamma_H^{(1)}$ electron flow from M1 to a single-populated HOMO. In this transmission mode, the probability of the P* excited state of the molecule is the highest. Therefore, the electroluminescence power, $W \sim P^*$ is maximal. As a result, if the electric energy $|e|V$ exceeds the HOMO-LUMO gap $\varepsilon_L - \varepsilon_H$, a stable photoactive state of the fluorophore occurs. This state proceed to the ground state with the emission of the quantum of light with frequency $\hbar\omega = \varepsilon_L - \varepsilon_H$, and then recovers due to the transition of an electron from HOMO to M2 and another electron from M1 to LUMO. We have shown that, although the potential of the gate (V_g) has little effect on the HOMO-LUMO gap size, it changes the charge states of the molecule. These states, as well as charge-neutral ones, are involved in the kinetics of transitions and thus are responsible for the formation of the photoexcited state of fluorophore. As a consequence, turning on the potential of the base can change the quantum yield of electroluminescence by an order of magnitude.



STRUCTURAL AND OPTICAL STUDY OF GLUTATHIONE-CAPPED Ag–In–S NANOCRYSTALS

B.V. Lopushanska[a], Y.M. Azhniuk[a,b], D. Solonenko[c], V.V. Lopushansky[b],
I.P. Studenyak[a], D.R.T. Zahn[c]
[a] *Uzhhorod National University. 46 Pidhirna Str., Uzhhorod 88000, Ukraine*
e-mail: lopushanska5@gmail.com
[b] *Institute of Electron Physics, Nat. Acad. Sci. Ukr.,*
21 Universytetska Str., Uzhhorod 88017, Ukraine
[c] *Semiconductor Physics, Chemnitz University of Technology, Chemnitz 09126, Germany*

In the recent years Ag–In–S water-soluble nanocrystals (quantum dots) produced by colloidal synthesis are intensely studied in view of their intense broadband luminescence in the visible spectral range as well as possible applications in light sources, solar cells, photocatalysis and biology [1, 2]. Here we report on the synthesis and optical characterization of size-selected non-stoichiometric Ag–In–S nanocrystals (NCs) obtained from $AgNO_3$, $InCl_3$, and Na_2S aqueous solutions in the presence of glutathione (GSH). The NC size selection was carried out by repeated fractioning of the colloidal solutions by precipitation at 4000 rpm in the presence of a non-solvent (2-propanol). Several series of size-fractioned colloidal NC solutions were prepared for different $[Ag^+]:[In^{3+}]$ and $[Ag^+]:[S^{2-}]$ component ratios in the reaction mixtures.

The Ag–In–S/GSH NCs produced were characterized by optical absorption and photoluminescence (PL) (StellarNet spectrometer) as well as X-ray diffraction (Rigaku Smartlab) and Raman spectroscopy (LabRAM, λ_{exc} = 325, 488, and 515 nm). The optical absorption edge and PL maxima of the size-selected NC series exhibit a clear size-dependent shift. Band gap values were determined from Tauc plots for direct allowed optical transitions. The average NC size was estimated from the correlation between the band gap and the NC size based on optical absorption and TEM data [1] as well as XRD data.

The effects of $[Ag^+]:[In^{3+}]$ and $[Ag^+]:[S^{2-}]$ component ratios in the reaction mixture on the optical absorption and PL parameters of the NCs formed are discussed. The analysis of the Raman spectra of the Ag–In–S NCs obtained versus the $[Ag^+]:[In^{3+}]$ and $[Ag^+]:[S^{2-}]$ component ratios in the reaction mixture enabled us to assign the observed Raman features to the corresponding bond vibrations.

[1] A. Raevskaya, V. Lesnyak, D. Haubold, V. Dzhagan, O. Stroyuk, N. Gaponik, D.R.T. Zahn, A. Eychmüller, J. Phys. Chem. C **2017**, 121, 9032–9042.
[2] O. Stroyuk, A. Raevskaya, F. Spranger, O. Selyshchev, V. Dzhagan, S. Schulze, D.R.T. Zahn, A. Eychmüller, J. Phys. Chem. C **2018**, 122, 13648–13658.

COMPLEX PERMITTIVITY OF EPOXY COMPOSITES WITH CARBON NANOTUBES AND TiO_2 IN MICROWAVE RANGE

O.V. Lozitsky[a], L.L. Vovchenko[a], L.Y. Matzui[a], V.V. Zagorodnii[b], V.V. Oliynyk[b]
[a] *Department of Physics,* [b]*Department of Radiophysics, Electronics, and Computer Systems*
Taras Shevchenko National University of Kyiv, Volodymyrska str., 64/13, Kyiv, 01601, Ukraine
e-mail: Olozitsky@gmail.com

Titanium oxide (TiO_2) composite materials (CMs) has been shown to interact strongly with microwave radiation when used in combination with conductive phase [1]. Here the microwave properties of L285 epoxy, filled with 1-5 wt. % of carbon nanotubes (CNT) and 35 wt. % of TiO_2 powder, have been investigated.

The s-parameters spectra have been measured and the complex permittivity values calculated in the frequency range 1-67 GHz using waveguide spectroscopy and Nicholson-Ross method, respectively. The dielectric constant was observed to increase non-monotonously with CNT content, though frequency dependencies are similar (Fig. 1a).

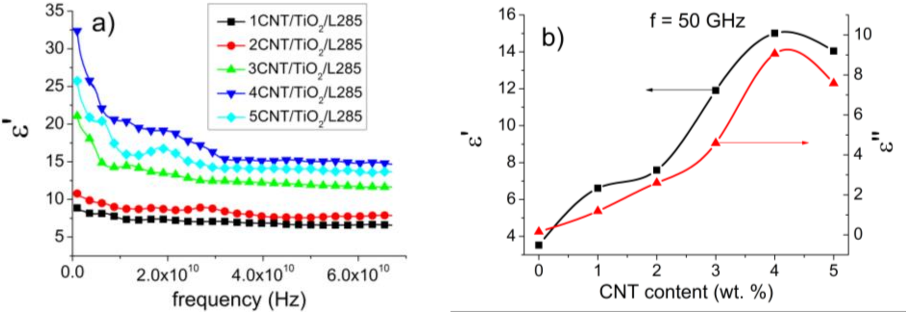


Figure 1. Real (a) and imaginary (b) parts of permittivity of epoxy CMs with CNT/TiO_2 filler.

Most notable feature of the complex permittivity versus CNT content (Fig. 1b) is correlating dependence of imaginary part of permittivity with real part, even at high CNT content, suggesting there are multiple factors taking part in its formation, with particle dispersion across the matrix, size of the conductive clusters and interfacial polarization creating local extremum in permittivity CNT content dependence, though the general increase of permittivity with CNT content is expected. It is possible that the mentioned factors can be exploited to obtain high permittivity and low loss materials with CNT/TiO_2/epoxy CMs.

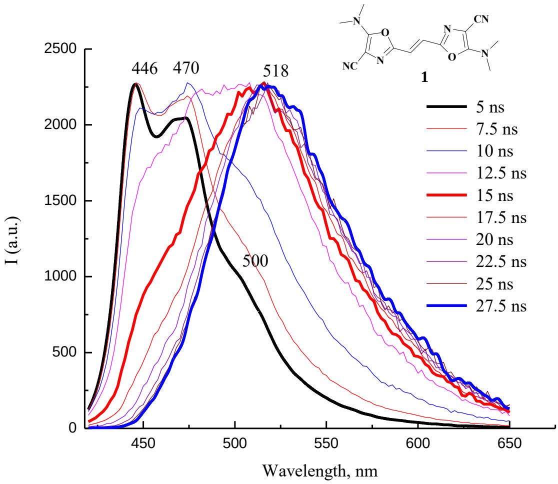
[1] Green M, Chen X, Recent progress of nanomaterials for microwave absorption, *Journal of Materiomics*, **2019**, 5, 503-541.

STUDY OF EXCITED STATE RELAXATION IN SUBSTITUTED POLYENES BY TIME-RESOLVED ELECTRON SPECTROSCOPY (TRES)

K. O. Maiko[a], D. O. Merzhyievskyi[b], O. V. Shablykin[b], Yu. P. Piryatinski[c], I. M. Dmytruk[a],
Ya. O. Prostota[b], N. V. Obernikhina[d], O .D. Kachkovsky[b], V. S. Brovarets[b]
[a]Taras Shevchenko National University of Kyiv , 60 Volodymirska Str., 03127, Kyiv, Ukraine
[b]V.P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry of the NASU,
1, Murmanskaya Str, Kyiv, 02660, Ukraine
[c]Institute of Physics NASU, 46 Nauki Ave., 03039 Kyiv, Ukraine
[d]O.O. Bogomolets National Medical University, 13 T. Shevchenko Blvd., Kyiv, 01601, Ukraine
e-mail: maiko_kate@ukr.net (Kateryna O. Maiko)

In the neutral polyenes, presented in our investigation, with their equalized atomic charges and alternated bond lengths, the excitation causes firstly the change of the bond lengths; thus, the polyenes demonstrated the considerable Stock’s shifts. Change of bond lengths is a result of relaxation in the excited state and can be accompanied by appreciable spectral effects.

The changes in the time-resolved electronic spectra (TRES) could be strictly connected with the changes in the electron structure when going from ground state to the excited spectra. We have restricted only by the low temperature spectra in the strong polar solvent, when the conformational (vibrational) transitions are no possible. The measured TRES of neutral polyene with 1,3-oxazole terminal groups shown in figure.



One can well-defined see that fluorescence spectrum of molecule undergo essential transformation during life-time flow. The appreciable regular changes in time-resolved spectra points unambiguously on the complicated relaxation path of the dye molecule 1 in the excited state, including the appearance of the speed component and appearance of additional long-time component. The appearance of the fast component is directly connected with the considerable redistribution of the electron densities at the carbon-carbon bonds upon the unchanged geometry; it disappears after the finished symmetrical relaxation; then time-resolved spectra correspond to the steady fluorescence. Also, in report, the quantum-chemical treatment of relaxation path is discussed, in detail.

ELECTRICAL AND THERMAL PROPERTIES OF EPOXY COMPOSITES FILLED WITH CARBON NANOTUBES AND INORGANIC PARTICLES

Len T.A., Vovchenko L.L., Turkov O.V., Lozitsky O.V., Matzui L.Yu.
[a] *Taras Shevchenko National University of Kyiv, Departments of Physics, Volodymyrska Str., 64/13, Kyiv, 01601, Ukraine*
e-mail: Olozitsky@gmail.com

The paper presents the results of the investigations of temperature dependencies of the electrical and thermal conductivity of epoxy composites (CMs) with two-component fillers, multiwall carbon nanotubes (MWCNT)/TiO_2 and MWCNT/carbonyl iron (Fe). The MWCNT concentration ranged from 1 to 5 wt. %, while the content of the second component was constant and was 35 wt.% TiO_2 and 30 wt.% Fe. It was found that the addition of the second type of filler along with MWCNT leads to an increase of the percolation threshold compared to MWCNT/epoxy CMs: C_{Cr}=0.3 wt.% for MWCNT/epoxy, 0.9 wt.% for CM MWCNT/TiO_2/epoxy and 2.2 wt.% for MWCNT/Fe/epoxy (Fig. 1a). On the other hand, when the MWCNT content is higher than 3 wt.%, the conductivity of CMs with the two-component fillers is much higher than that of the MWCNT/epoxy.

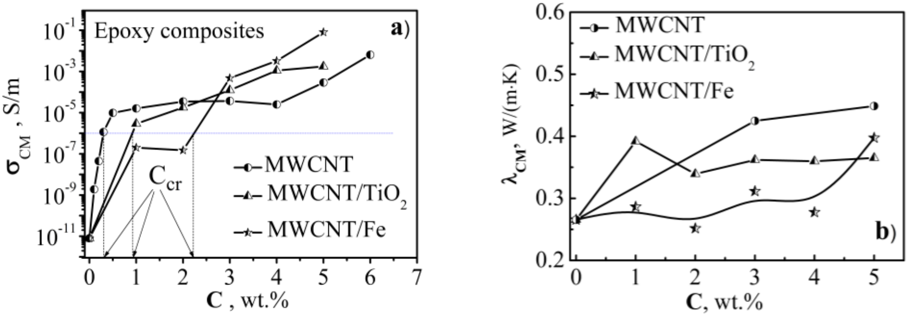


Figure 1. Electrical (a) and thermal (b) conductivity for epoxy CM versus MWCNT content.

The temperature dependencies of the electrical resistance of these CMs indicate a tunneling mechanism of electrical conductivity, and the ratio ρ_{77}/ρ_{290} is equal to 1.25-1.33.

The experimental data of thermal conductivity of CMs (Fig. 1b) show that adding of two-component fillers MWCNT/TiO_2 or MWCNT/Fe into epoxy promotes smaller changes in thermal conductivity compared to two-phase MWCNT/epoxy composites. The low thermal conductivity of CNT-based CMs may be explained by the high values of the thermal interface resistance, especially in the case of CMs with two-component fillers.

LOW ENERGY ELECTRON INDUCED PLASMON EXCITATIONS IN THE W (100)

M. O. Vasylyev, I. M. Makeeva, V. M. Kolesnik, V. I. Patoka
G.V. Kurdyumov Institute for Metal Physics, N.A.S. of Ukraine,
36 Academician Vernadsky Boulevard, UA-03142 Kyiv, Ukraine
e-mail: mak0506@ukr.net

The modern progress in such priority scientific directions as nanophysics and nanotechnology are impossible without obtaining quantitative information about physical–chemical properties from the nanometer near surface region of the materials. Electron Energy Loss Spectroscopy (EELS) can be used for the investigation of the electronic states densities, plasma oscillations of the free-electron gas, crystal structure, and element composition in the near surface layers of the solid. EELS locality is conditioned by small mean free path of the emitting electrons with respect to the inelastic interaction which is determined by their kinetic energy and is in the limits ~ 0.2 to ~ 5.0 nm, depending on the primary electron energies E_0. The main types of the losses are the losses concerned with ionization of the core-electron levels, excitation of both the surface and bulk plasmons, and interband transitions.

The aim of this work is to study the plasmon excitations in the EELS spectra, obtained during irradiation of the W (100) surface by the primary electron beam in the low energy range. The study of the atomically pure faces of the metal single crystals under ultrahigh vacuum allows to increase the reliability of the data and compare experimental results with existing theories and theoretical models developed for ideal crystals with the free surface. All measurements were performed in the ultrahigh vacuum chamber equipped with a four-grid quasispherical energy analyzer of the LEED–AES type, electron and ion guns [1]. Residual gas pressure in the chamber was about 10^{-7} – 10^{-8} Pa. The energy resolution of the four-grid analyzer is $\Delta E \approx$ 0.1% - 0.2% in the primary electron energies E_0= 50–600eV.

The energies of the surface (E_s) and bulk (E_b) plasmons were measured as the function of the primary electron energy (E_0) in the initial state, after heating in the temperature range 500-1600^{0}C, and after exposure to oxygen and irradiation with argon ions. The averaged values of the surface and bulk plasmon energies and their ratios, the concentration of conduction electrons involved in plasma oscillations, and the relative change in the interplanar distance are calculated. Deviation of the plasmon excitations from the theoretical value calculated in the free-electron gas model was found. An experiment showed that the plasmon energy relation E_b / E_s exceeds the theoretical values, which is apparently due to the fact that the free-electron gas model does not take into consideration real physical–chemical state of the surface.

.

1. M. A. Vasil’ev and S. D. Gorodetsky, Vacuum, 1987, 37, 723-728.

SURFACE PROPERTIES OF METAL FILLED COMPOSITE BASED ON POLYMER BLEND

Misiura A.[a], Mamunya Ye.[b], Prochazka M.[c], Omastova M.[c], Kulish M.[a], Pylypenko A.[b]

[a] *Taras Shevchenko National University of Kyiv, Physics faculty, 4 Prospekt Hlushkova, Kyiv 03022, Ukraine; e-mail: andrii_misiura@ukr.net*

[b] *Institute of Macromolecular Chemistry of National Academy of Sciences of Ukraine, 48 Kharkivske shausse, Kyiv 02160, Ukraine; e-mail: ymamunya@ukr.net*

[c] *Polymer Institute, Slovak Academy of Sciences, Dubravska cesta 9, 845 41 Bratislava, Slovakia; e-mail: maria.omastova@savba.sk*

Conductive polymer composites are widely used in various fields of microelectronics. At their application not only electrical properties, but also surface characteristics are important. The composition of the composites affects both the conductivity parameters and the surface properties. The change of conductive filler content (Fe) leads to the varying of conductivity.

Conductive composites are based on polymer blend of the co-polyamide master batch which involved 40 vol.% Fe (CPA-Fe) and pure polypropylene (PP) component. When the CPA-Fe increases from 0 to 100%, the Fe content increases from 0 to 40 vol.%, accordingly the PP component is reduced from 100 to 0 %.

The method of contact angle measurement was used. As testing liquids, we applied water (*W*) and diiodomethane (*D*) with known surface parameters.

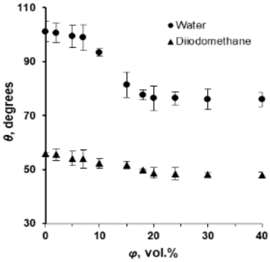


Fig.1. Contact angle dependences on concentration of the PP/CPA-Fe composite.

The dependence of the contact angle θ for both liquids on filler content is shown in Fig. 1, the value of the contact angle for *W* (θ_W) is much higher than for *D* (θ_D), although behavior of both dependencies is similar. The highest values of θ_W=103° are observed for pure PP that indicates the high hydrophobic properties of the composite surface. As it can be seen, there are three different regions in the concentration dependence, which corresponds to the morphology of the composite. The biggest changes in values of θ are observed in the concentration range from 7 to 18-20 vol.% of Fe, which corresponds to the phase inversion region where PP and CPA-Fe phases are co-continuous and provide the transition from PP-matrix to CPA-Fe matrix structures. The change of θ correlates well with alteration of the composite conductivity.

CARBON NANOTUBES AS MODIFIERS OF PROPERTIES OF MATERIALS

H.Yu. Mykhailova
G. V. Kurdyumov Institute for Metal Physics of the N.A.S. of Ukraine, 36 Academician Vernadsky Boulevard, UA-03142 Kyiv, Ukraine
e-mail: mihajlova.halina@gmail.com

Carbon is striking in its variety of properties. Each of its modifications and alotropic forms opens new possibilities from its applications. Carbon nanotubes, that have unusual physical and mechanical properties, have been actively attracting the attention of scientists since their discovery. Their introduction into a metal or polymer matrix also contributes to a cardinal change in properties.

The introduction of 3.5% CNTs into the polymer matrix contributes to the appearance of electrical conductivity, mechanical mixing with metal particles is increase electrical conductivity by an order of magnitude.

The presence of defects also significantly affects the properties of such materials. Defects in CNTs can be formed both during synthesis and under external influence, for example, radiation exposure, created defects distort the structure, can make crosslinking of CNTs, which changes their electronic characteristics.

The electromechanical properties of mechanical mixtures of metal-carbon nanotubes were investigated. It is shown that the addition of CNT to metallic particles of copper, titanium, $LaNi_5$ increases the conductivity at a certain concentration of CNTs, which is caused by the exchange of electrons between CNTs and metal particles.

FORMATION OF DONOR-ACCEPTOR COMPLEXES IN FULLERENE SOLUTIONS

Nagorna T.V.[a,b], Bulavin L.A.[a], Chudoba D.[b,c,d]
[a] *Taras Shevchenko National University of Kyiv, Hlushkova Avenue 4, Kyiv 03127, Ukraine*
[b] *Joint Institute for Nuclear Research, Joliot-Curie 6, Dubna 141980, Russia*
[c] *Adam Mickiewicz University, Umultowska str. 85, Poznan 61-614, Poland*
[d] *St. Petersburg State University, Ulyanovskaya str. 3, St. Petersburg 198504, Russia*
e-mail: great.lond@gmail.com

Since fullerenes were discovered potential applications of fullerene solutions in various fields including electronics, optics, cosmetics, and pharmaceutics were intensively studied [1-3]. Due to their unique molecular structure (Fig.1) fullerenes exhibit unusual macroscopic properties such as high electrical conductivity, high heat conductivity, thermal and concentration dependence of optical parameters, anomalous solubility etc. Fullerene solutions also demonstrate the solvatochromic effect, which can be observed with a slight change in the polarity of the system (Fig.2).

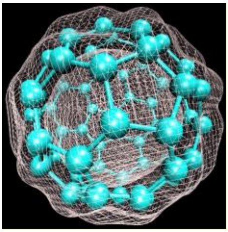


Fig. 1. C_{60} with isosurface of ground state electron density as calculated with density functional theory.

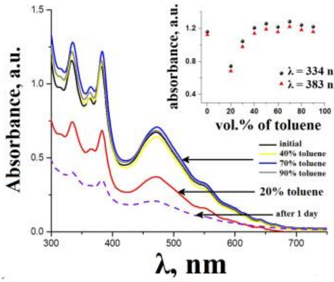


Fig. 2. UV–vis spectra of the C_{70} / NMP solution with various ratio of toluene. The inset demonstrates dependence of the extinction coefficient at two different wavelengths versus the toluene volume fraction in the mixture [4].

Solvatochromic effect can be related to the appearance of donor-acceptor complexes between fullerene and solvents molecules on the cluster surface. In the work were studied fullerenes C_{60} and C_{70} in toluene and / or N-methyl-2-pirrolydone solutions. The processes of formation of complexes with charge transfer are described. The processes of cluster formation were also studied in order to exclude their influence on changes in the absorption spectra.

[1] L. Wang, *J. Phys. Chem. Solids*, **2015,** 84, 85-95.
[2] M. Xing, R. Wang, J. Yu, Int. J. *Refrigeration*, **2014,** 40, 398-403.
[3] S. Afreen, K. Muthoosamy, et al., *Biosensors and Bioelectronics*, **2015,** 63, 354-364.
[4] T. Nagorna, M. Kuzmenko, O. Kyzyma et al., *Journal of Molecular Liquids*, **2018**, 272, 948-952.

PECULIARITIES OF THE SPECTRAL PROPERTIES OF BORON-CONTAINING DYES IN THE AQ3 MATRIX

O.M. Navozenko[1]*, V.M. Yashchuk[1], M.Yu. Losytskyy[1], A.P. Naumenko[1], I.Yu. Doroshenko[1], Yu.L. Slominskii[2], D. Gudeika[3]
[1]*Faculty of Physics, Taras Shevchenko National University of Kyiv, 64/13, Volodymyrska Street, 01601 Kyiv, Ukraine*
[2]*Department of Colour and Structure of Organic Compounds, Institute of Organic Chemistry, National Academy of Sciences of Ukraine, 5 Murmanska str., 02660 Kyiv, Ukraine*
[3]*Department of Polymer Chemistry and Technology, Kaunas University of Technology, Radvilenu pl. 19, LT-50254, Kaunas, Lithuania*
e-mail: a_navozenko@ukr.net

In order to develop the technologies for the fabrication of high effective light-emitting devices, much attention is being paid to the study of thin composite organic films. Most important role in composite material efficiency belongs to the impurity molecules. That's why the attention of the researches is focused on synthesis of new effective molecules. In this work the optical properties of boron-containing molecules which can be used as such impurities have been investigated. The absorption spectra of these dyes have been analyzed for dye molecules in solution, in solid Alq3 thin films and single component films of pure dyes.

Comparing the absorption spectra of solutions and solid Alq3 films, it can be seen that positions of absorption lines coincide only if the impurity concentration in the Alq3 matrix not more several percent. The absorption spectra maxima in single-component films are shifted relative to the maxima in the solution. We assume that this effect is caused by the aggregation of impurity molecules or the intermolecular interaction. The long-wavelength maximum in a single-component film is shifted to the long-wavelength region and is much broader than the corresponding maximum in the solution. The short wavelength maxima in some dyes is broadened and shifted to the short-wavelength region. It was shown that in a single-component film the spectra are changed in a similar way in comparison with solutions because both monomers and aggregates of molecules are present, and also these spectrum changes may be induced by the intermolecular interaction in the film.

FIELD-CONTROLLED ELECTRON TRANSPORT IN CHOLESTERIC LIQUID CRYSTAL – CARBON NANOTUBES COMPOSITE

Yu.I. Olenych, Yu.Yu. Horbenko, O.I. Aksimentyeva, I.B. Olenych, I.D. Karbovnyk
Ivan Franko National University of Lviv, 50 Dragomanov Street, 79005 Lviv, Ukraine
e-mail: iolenych@gmai.com

Nowadays the promising direction for nanotechnology development is the creation of nanocomposite materials possessing new functional properties, in particular, nanosystems based on carbon nanotubes (CNTs) incorporated in a dielectric matrices [1,2]. Usually, the content of CNTs in composites determines their conductive, heat-conductive and mechanical properties. The electrical charge in the dielectric – CNTs composites is transferred through a network of conductive nanotubes. Therefore, an important condition for the electrical conductivity of such composites is the formation of percolation clusters of CNTs. The study of percolation phenomena in the CNT system shows a significant influence of the nanotube predominant orientation on the threshold value of percolation [3]. On the other hand, the use of liquid crystal as a host medium makes it possible to manipulate CNTs and control their orientation [4].

In this work, cholesteric liquid crystal – CNTs composites were obtained and their electrical properties were studied in AC mode. We have found that nanocomposites show a decrease in internal resistance with increasing the frequency from 25 Hz to 1 MHz. In addition, the electrical characteristics of our nanosystems depend significantly on the composite content. Increasing the mass concentration of the CNTs from 1 to 8% causes a decrease in the composite resistance by four orders of magnitude: from several GOhm to hundreds kOhm. The increase in conductivity is associated with the formation of percolation clusters in the CNTs network. Under the influence of an external electric field, the composite resistance was decreased, which is likely related to an increase in the probability of percolation in the oriented nanotube system. The greatest relative change in resistance was observed for the composite with 2–4% CNTs content. Obtained results can be used to create new kinds of electronic devices.

[1] Francis R., Joy N., Aparna P., Vijayan R. *Polymer Rev*. 2014, **54**, 268.

[2] Karbovnyk I., Olenych I., Aksimentyeva O., Klym H., Dzendzelyuk O., Olenych Yu., Hrushetska O. *Nanoscale Res Lett*. 2016, **11**, 272.

[3] Olenych Yu., Karbovnyk I., Klym H. *In: Proceedings of 14th International Conference on Perspective Technologies and Methods in MEMS Design*, 2018, 48.

[4] Massey M.K., Kotsialos A., Volpati D., Vissol-Gaudin E., Pearson C., Bowen L., Obara B., Zeze D.A., Groves C., Petty M.C. *Scientific Reports*, 2016, **6**, 32197.

NANOCOMPOSITES OF CONDUCTING POLYMERS AS ACTIVE LAYERS FOR ELECTRONIC GAS SENSORS

A. Pud[a], N. Ogurtsov[a], O. Kukla[b], Yu. Noskov[a], J.-L. Wojkiewicz[c], V. Bliznyuk[d], A. Mamykin[b], I. Myronyuk[a]
[a] *V.P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry of NAS of Ukraine, 50 Kharkivske shose, Kyiv, 02160, Ukraine.*
[b] *V.E. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine, 45 Prospekt Nauky, Kyiv, 03028, Ukraine*
[c] *IMT Lille-Douai, Univ. Lille, SAGE-Department, Sciences de l’Atmosphère et Génie de l’Environnement, F-59000 Lille, France*
[d] *Environmental Engineering & Earth Sciences, Clemson University, Clemson, SC, USA*
e-mail: alexander.pud@gmail.com; pud@bpci.kiev.ua

Our current interest to nanocomposites of intrinsically conducting polymers (ICP) is specifically related to one of their important capabilities namely to efficient performing as sensitive elements in electronic gas sensors. In fact, this capability stems from unification of electrophysical and physico-chemical properties as well as of structure/morphology specificity of ICP and other component(s) in one nanostructured material. In this report we will consider how we can govern and enhance this unique combination /set of such sensing materials. In particular, as most important factors of influence, especially, in case of core-shell nanocomposites, we will discuss:

- Conditions of synthesis, formation and treatment/modification of the nanocomposite;
- Physico-chemical interactions both of the monomer and the forming ICP layer/shell with other components of the nanocomposite;
- Nature, size and number of core nanoparticles
- Dopant nature;
- Doping conditions;
- Oxidation degree and charge carriers;
- Conditions for intra and intermolecular charge transfer;
- Conformation of ICP chains;
- Morphology and structure of ICP layer/shell;
- Controllable conditions of preparation of sensor layers on electrodes.

FEATURES OF CYANINE AGGREGATES FORMATION IN NANOPOROUS MATRICES

I. Ropakova, A. Sorokin, I. Bespalova, S. Yefimova, Yu. Malyukin
Institute for Scintillation Materials of NAS of Ukraine
60 Nauky Ave., Kharkiv, 61072, Ukraine
e-mail: ropakova@isma.kharkov.ua

In modern optics, the most popular destinations are optoelectronics, photovoltaics, optical methods of recording and processing of information. They are inseparably linked with nanophotonics where a special role is played by organic fluorescent nanostructures, such as conjugated polymers and J-aggregates, due to their unique spectral properties, relative ease of manufacture and enormous opportunities of functional design. The photophysical characteristics of J-aggregates, such as narrow absorption band, resonant fluorescence, giant third-order susceptibility, high oscillator strength, etc., are dramatically different from those of the individual molecules forming the aggregate. Such optical properties of J-aggregates are explained by strong interaction between the molecules and their ordering within the aggregates resulting in the delocalization of electronic excitations over certain molecules on the chain with Frenkel exciton formation. As a result, a red-shifted exciton band (J-band, the “face-to-tail” arrangement) appears thought depending on a molecular packing in the aggregate chain a blue-shifted exciton band (H-band, the “face-to-face” arrangement), or both J- and H-bands (the “herringbone” arrangement with two molecules in the chain unit resulting in Davydov-splitting) can be also observed. The special feature of J-aggregates is a close correlation between J-aggregate excitonic properties and structure that opens up possibilities for the manipulation of J-aggregate optical characteristics by changing the condition of nanocluster formation.

J-aggregates could change their structure in different media, especially solid nanostructured materials like nanoporous matrices or polymer films. In the present report, we demonstrate a possibility of J-aggregates usage as the probe for nanostructured materials. As the probing tool, the exciton delocalization length has been used as well as the lifetime. It has been shown direct dependence of the exciton characteristics of the J-aggregates on the specific features of nanoporous matrices including TiO_2 and anodic aluminum oxide ones.

ESTIMATION OF DIPOLE MOMENTS FOR THE PHENALENONE DYES IN LIQUID AND POLYMER POLAR MEDIA

T.V. Bezrodna[a], L.F. Kosyanchuk[b], O.M. Roshchin[a], V.I. Bezrodnyi[a],
G.V. Klishevich[a], V.I. Melnyk[a]
[a] *Institute of Physics NASU, 46 Nauki av., Kyiv 03680, Ukraine*
[b]*Institute of Macromolecular Chemistry NASU, 48 Kharkivske av., Kyiv 02160, Ukraine*
e-mail: a_roshchin@ukr.net

Optical phenomena, observed in organic dyes, such as fluorescence and selective absorption of light attract attention of the researchers in different fields of science and technology. Requirements for their applications determine a use of various solvents, in particular, liquids, polymers, liquid crystals and sol-gel glasses. Knowledge of dipole moments for the electron-excited molecules of the dyes is often important for the development of nonlinear optical materials, interpretations of excited state types, and also for the investigations of any photochemical transformations.

This work is aimed at the determination and comparison of dipole moments, investigations, prediction and improvement of photophysical properties for the three phenalenone dyes (6-amino-1-phenalenone, 2-chloro-6-(3-methylamino)-1-phenalenone, 2-chloro-6-(3-hydroxypropylamino)-1-phenalenone) in liquid solvents (butyl acetate, ethyl acetate, dichloromethane, ethanol, acetonitrile) and polymer matrices (polyurethanes of different oligoether and diisocyanate components), depending on the medium polarity characteristics. The differences in polarity of the used polyurethanes are specified by the chemical structure of selected initial compounds for the polymer synthesis and conformation flexibility of the polymer chains.

The solvatochromic phenomena for the phenalenone dyes in liquid and polymer matrices of different polarity have been investigated by means of the spectroscopic analysis. Based on Bakshiev's and Kawski-Chamma-Viallet's theoretical considerations, the dipole moments of the phenalenone molecules in the ground and excited states have been calculated for the liquid solvents and polymer matrices. Obtained linear dependencies of Stokes shift on the media polarity function in the both cases indicate a common type of intermolecular interactions in these systems. The larger values of dipole moments in excited states prove a positive solvatochromic effect for these molecules, which appears as a bathochromic shift of the spectral bands. The data for the dipole moments, determined for the phenalenone molecules in the polyurethane matrices are in a good agreement (not worse than 10%) with the ones, obtained for polar liquid solvents.

Thus, polyurethane polymer matrices of high polarity can serve as appropriate media for the determination of dipole moments for the dye molecules by a solvatochromism method.

THE STUDY OF TiO_2/SnO_2 COMPOSITION AFTER IT SONOCHEMICAL AND MECHANOCHEMICAL TREATMENT

Sachuk O.V., Zazhigalov V.A., Diyuk O.A., Tsyba M.M.
Institute for Sorption and Problems of Endoecology, 13 General Naumov str., Kyiv, 03164, Ukraine
e-mail: Slena951@ukr.net

It is known that TiO_2/SnO_2 compositions are effective catalysts, photocatalysts, UV-sorbents, sensors, catalytic supports with unique properties which are different from individual oxides. Traditional methods of Ti-Sn-O preparation such as sol-gel, solvo/hydrothermal, thermal decomposition, precipitation don't allow to synthesize of effective photocatalytic systems. In this regard, in the work the ultrasonic treatment is a new eco-friendly and simple method which is allow to realize the synthesis of complex Ti-Sn-O compositions and nanocompositions from initial compounds and assess the degree of their transformation.

It is found that after ultrasonic (UST) and mechanochemical (MChT) treatment of TiO_2/SnO_2 = 1:1 composition leads to anisotropic deformation of tin oxide and decrease of particle sizes in SnO_2 (as a dominant reflex) from 65 to 22 nm. The FT-IR spectroscopy studies show that after modification the shifting of absorption bands of stretching and deformation Ti-O bond from 1345 and 1074cm^{-1} to 1354 and 1086 cm^{-1} respectively was observed. The disappearance of stretching vibration Sn-O-Sn and Sn-O bonds at 613 and 536 cm-^{1} respectively and absorbance band of Ti-OH bond at 1165 cm^{-1} occurs.

According to BET results the ultrasonic treatment of the samples are characterized by an increase in the specific surface (from 2 to 8 m^2/g), total pore volume (from 0.02 to 0.07 cc/g) and a change in the porous structure, namely - mesopores formation.

The studies of surface morphology and structural properties of Ti/Sn composition it was found that after treatment the formation a lot of agglomerated nanoparticles occurs.

The photocatalytic properties of studied composition in degradation reaction of organic dyes (safranin T) show that sono- and mechanochemical treatment accompanied by increase of photocatalytic activity in this reaction under UV- and visible light (Table 1).

Table 1

Photocatalytic activity of TiO_2/SnO_2 samples in safranin T degradation ($K_d \times 10^4$,s^{-1})

Parameter	**initial**	**UST**	**MChT**
UV-light	1.02	6.85	5.35
Visible irradiation	1.84	5.53	4.80

Catalytic properties of this system in selective ethanol oxidation reaction showed that synthesized samples by mechanochemical and ultrasonic rout demonstrate the promising results in ethanol oxidation to hydrogen. There are no carbon dioxide and selective of hydrogen formation is about 40%.

SILVER NANOPARTICLES EFFECT ON THE SENSITIZATION OF DYE-SENSITIZED SOLAR CELLS

Temirbayeva D.A.[a], Seliverstova E.V.[a], Ibrayev N.Kh.[a], Ishchenko A.A.[b]
[a]*Buketov Karaganda State University, Universitetskaya 28a, 100028, Karaganda, Kazakhstan*
[b]*Institute of Organic Chemistry, NAS of Ukraine, Kyiv, Murmanskaya str. 5, 02660, Kiev-94, Ukraine*
e-mail: imnph@mail.ksu.kz

Currently, many research groups are working to improve the characteristics of solar cells. Increasing the efficiency of solar energy conversion by solar cells can be achieved with using of phenomenon of plasmon resonance of metal nanoparticles (NPs), as well as the Förster resonance energy transfer (FRET).

In this work, we studied the effect of plasmon resonance of silver NPs on the efficiency of spectral sensitization of TiO_2 semiconductor films in dye-sensitized solar cells (DSSC) based on donor-acceptor (DA) dye pairs. Rhodamine 6G (R6G) and the cationic polymethine dye K1 were chosen as energy donors, and the cationic polymethine dye K2 was the acceptor [1]. The photovoltaic parameters of solar cells, sensitized by neat donor or neat, and separately by DA pairs in the presence and without Ag/TiO_2 core/shell NPs were measured (Table).

Table 1 – Photovoltaic parameters of DSSC with DA pairs and neat dyes without and in the presence of Ag/TiO_2 NPs (concentration of 1 wt% relative to TiO_2)

Dye	Sample	I_{sc}, mA/cm^2	V_{oc}, mV	FF	Efficiency, %
R6G	TiO_2	0.04	206	0.46	0.038
	TiO_2/Ag	0.05	234	0.46	0.054
K1	TiO_2	0.28	352	0.182	0.18
	TiO_2/Ag	0.47	403	0.12	0.32
K2	TiO_2	0.04	215	0.575	0.07
	TiO_2/Ag	0.06	246	0.56	0.06
R6G+K2	TiO_2	0.07	224	0.35	0.055
	TiO_2/Ag	0.07	328	0.40	0.092
K1+K2	TiO_2	0.40	441	0.20	0.35
	TiO_2/Ag	0.66	445	0.16	0.47

In the presence of Ag/TiO_2 NPs efficiency of solar cells was increased. The measurements showed that in the R6G-K2 pair the growths in the efficiency is mainly due to the expansion of the spectral sensitivity of the semiconductor film when it is doped with Ag/TiO_2 NPs. For the K1-K2 pair, the final efficiency is greater than the sum of the individual components, which may indicate an additional contribution of FRET between dye molecules, as well as the influence of the plasmon in the optical properties of the dyes.

[1] E. Seliverstova, D.Temirbayeva, N. Ibrayev, A. Ishchenko. *Theor. Exp. Chem.*, **2019**, 55, 115-124.

ANALYSIS OF THE PROPERTIES OF METALLOORGANIC COMPOUNDS WITH THE Fe^{3+} NANOPROBES BY EPR METHOD

Shapovalov V.A.[a*], Aksimentyeva E.I.[b], Shavrov V.G.[c], Koledov V.V.[c],
Shapovalov V. V.[d], Tkach V.I.[a]

[a]*A. Galkin Donetsk Institute for Physics and Engineering, Nauki ave. 46, Kyiv, Ukraine*
[b]*Ivan Franko National University of Lviv, Universitetskaya str. 1, Lviv 79000, Ukraine*
[c]*Kotelnikov Institute of Radio-engineering and Electronics of RAS, Moscow, Russia*
[d]*Math for America Master Teacher, MfA, 160 Fifth Ave, 8th floor, NY, NY 10010, USA*
**e-mail: vashapovalov1@mail.ru*

Metalloorganic substances like sodium salt $Na[FeO_6(C_{10}H_8N)_3]$, kaolinite, metalloproteins (ferritine, maltofer and Ferrum Lek) are studied. Metalloproteins are widely used in medical practice [1]. X-ray structural analysis of metalloorganic compounds containing the Fe^{3+} nanoprobes has been carried out. The study was accompanied by EPR testing with the use of model concepts describing temperature transformations of EPR spectrum [2]. X-ray diffractograms demonstrate the crystal structure of the substance (Fig. 1) and the presence of an amorphous structure. EPR testing was performed at a radiospectrometer within the temperature range of 4.2 - 300K, the frequency of 10 GHz. A change in the intensities of the lines of EPR spectrum and their mutual transfer is registered (Fig. 2). The dynamical characteristics of the nanoprobe environment is evaluated, namely, the height of the crystal field barrier at the location of the iron nanoprobe.

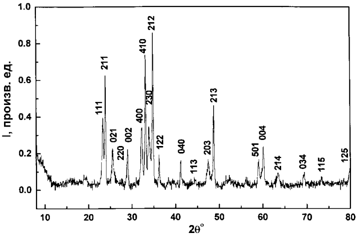


Fig. 1

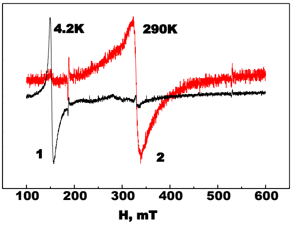


Fig. 2

Acknowledgments.

Many special thanks are extended to the staff of Math for America, especially to Professor John Ewing for inspiration, Ms. Courtney Allison and Mr. Michael Driskill for encouragement. The work was carried out within the framework of the state task with partial funding of the RFBR, grant No. 18-07-01320.

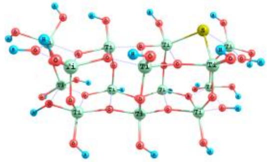
1. Saifutdinov R. G. Electron Paramagnetic Resonance in Biochemistry and Medicine. New York. 2019, pp. 276.

2. V.A. Shapovalov, V.V. Shapovalov, M. Rafailovich at al. Dynamic Characteristic of Molecular Structure of Poly(ortho-methoxyaniline) with Magnetic Probes. The Journal Physical Chemistry C. - 2013. -V. 117. - P. 7830−7834.

EFFECT OF NON-METAL ADMIXTURES ON THE ELECTRONIC STRUCTURE AND XPS CHARACTERISTICS OF TITANIA NANOPARTICLES

O.V. Smirnova, A.G. Grebenyuk, V.V. Lobanov
Chuiko Institute of Surface Chemistry, NAS of Ukraine, 17 General Naumov Str., Kyiv 03164, Ukraine
e-mail: olsmirnova2001@ukr.net

One of the promising materials for photocatalysis is pure or doped titanium dioxide TiO_2, the interest to it is due to its physicochemical properties. In addition, it is used as an effective photocatalyst for a number of chemical reactions and is widely appied to purifying water and air from toxic organic impurities. Also, to simulate the effect of atomic non-metal incorporation and isomorphic replacement of an O atom, anatase nanoparticles were represented as a set of clusters. The (001) face of a defect-free anatase surface was modeled earlier [1] by a cluster of the gross formula $Ti_{14}H_{22}O_{39}$. TiO_2 clusters doped with B, C, N, and S atoms were also considered. Different oxidation states of non-metal atoms were taken into account, so there can be boride and borate, carbide and carbonate, nitride and nitrate, sufphide and sulfate structures incorporated into the bulk of titania nanoparticles. The rearrangements of electron density distribution can be easily seen in related XPS spectra.



The calculations were carried out in the framework of the cluster approximation. using the density functional theory B3LYP method and the basis set 6-31G (d, p), using the PC GAMESS software package (FireFly version 8.2.0 by A. Granovsky).

All the oxygen atoms in a defect-free structure can be divided into some groups according to their coordination environment (2- and 3-coordinated ones) and the chemical nature of the second and third neighboring atoms [2]. Five peaks of O*1s* can be observed in the XPS spectrum calculated for the $Ti_{14}H_{22}O_{39}$ cluster model (about 521 eV). Each peak can be assigned to a specific type of O atoms.

Replacing oxygen atoms with admixture non-metal atoms complicates the spectrum. However, for example, in case of nitrogen insertion, 2 new peaks appear near 523 eV (522.87 and 523.28 eV) associated with 3-coordinated oxygen atoms.

Sulfur atoms in sulfide positions give S*2s* peaks near 215 eV whereas those in sulfate ones lead to appearance of peaks near 222 eV. The peaks of surrounding oxygen atoms in the first case form a group within 520.9 to 521.9 eV. Relative group of peaks for the oxygen atoms of sulfate admixture is within 520.8 to 522.7 eV. Analogous results have been obtained for other non-metal impurities.

In addition, cluster models of titanium dioxide were studied, including more than 21 Ti atoms. It has been shown that an increase in the number of atoms in the model does not contribute to improving the agreement between available experimental and theoretical data.

1. O. Smirnova, A. Grebenyuk, V. Lobanov, *Applied Nanoscience*, **2019**, 9(5), 1251-1254.
2. O. Smirnova, A. Grebenyuk, O. Linnik, V. Lobanov, *Springer Proceedings in Physics*, **2017**, 603-609.

CONTROL OF THE EXCITON SELF-TRAPPING IN LUMINESCENT MOLECULAR AGGREGATES

A. Sorokin, I. Grankina, S. Yefimova, Yu. Malyukin
Institute for Scintillation Materials of NAS of Ukraine
60 Nauky Ave., Kharkiv, 61072, Ukraine
e-mail: sorokin@isma.kharkov.ua

Supramolecular high-ordered assemblies, called J-aggregates, possess a number of unique spectral properties, which distinctly differ from those of the individual molecules, such as narrow absorption band, near-resonant fluorescence, high oscillator strength, giant third-order susceptibility, resonant, effective energy migration, etc. The specificity of J-aggregates is caused by electronic excitations delocalization over molecular chains and molecular (Frenkel) excitons formation due to translational symmetry and strong dipole-dipole interaction between molecules. However, the exciton properties of J-aggregates often differ from those of typical molecular crystals. First of all, it is associated with predominant one-dimensional J-aggregate geometry in solutions or two-dimensional geometry in films and on surfaces, while molecular crystals typically exhibit three-dimensional ordering. Another reason is a strong influence of significant configurational randomness of the J-aggregate environment leading to exciton localization, which plays a very important role in the optical dynamics.

Unique spectral properties make J-aggregates excellent candidates for novel photonic materials especially in the form of thin films, particularly, polymer films. Indeed, while in solutions J-aggregates often possess low photostability, in polymer films their stability becomes much higher. However, J-aggregate formation in polymer films has also disadvantages, such as low fluorescence quantum yield. One of the possible reasons is exciton self-trapping in a more rigid environment. The exciton self-trapping appears when the excitons localize themselves in the self-induced potential well caused by the large lattice distortion under the condition of strong exciton-phonon coupling.

The feature of J-aggregates is the strong dependence of exciton-phonon coupling, and hence the self-trapping efficiency, on the exciton coherence length. So, the control of the coherence length allows us to change the efficiency of the exciton self-trapping and, respectively, to influence the J-aggregate fluorescence. In the report, the methods of J-aggregates excitonic properties manipulation are discussed both for aqueous solutions and thin solid films.

TWO STAGE INTERCALATION OF MULTYWALL CARBON NANOTUBES WITH COBALT

D. O. Spylka[a], I. V. Ovsiienko[a], T. A. Len[a], L. Yu. Matzui[a], F. Le Normand[b],
T. L. Tsaregradskaya[a], G. V. Saenko[a]

[a]*Taras Shevchenko National University of Kyiv, Volodymyrska st. 64/13,*
Department of Physic, 01601, Kyiv,Ukraine
[b]*Institut de Physique et Chimie des Matériaux, 23 rue du Loess BP 43,*
67037 Strasbourg, France
e-mail: tsar_grd@ukr.net

The work is devoted to the problems of obtaining intercalated compounds based on multiwall carbon nanotubes (MWCNTs). The source MWCNTs have been produced by low-temperature catalytic decomposition of carbon monoxide. Intercalated MWCNTs specimens have been obtained by two-stage method with usage of C_8K as precursor [1]. At the first stage the MWCNTs intercalated with potassium according to equation $C + K \rightarrow C_8K$ was obtained by standard gas-phase method. At the second stage cobalt chloride in the interlayer space of MWCNTs was reduced to cobalt by the following scheme: $C_8K + MeCl_x \rightarrow C\text{-}Me + KCl$.

Figure 1 presents the fragment of X-ray diffraction pattern (a) and the typical TEM image (b) for synthesized cobalt intercalated MWCNTs.

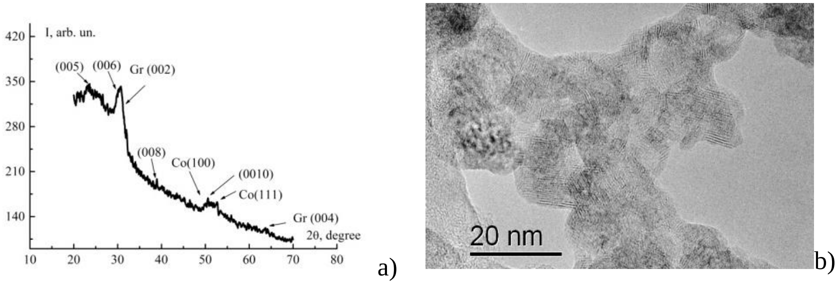


Figure 1. X-ray diffraction pattern (a) and TEM image (b) for cobalt intercalated MWCNT

As it follows from Fig. 1(a), the X-ray diffraction pattern contains a number of new bands, that correspond to the reflections from the layers of intercalate for intercalated compounds of the fourth stage. As can be seen from Fig. 1(b) a very heterogeneous structure of intercalated MWCNT is observed. In the work properties of cobalt intercalated MWCNTs are investigated, in particular, temperature dependences of magnetic susceptibility, electrical and magnetic resistance.

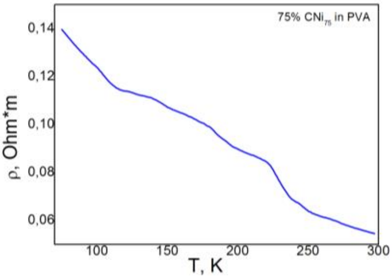
[1] I. Ovsiienko, L. Matzui, I. Berkutov et al. Magnetoresistance of graphite intercalated with cobalt., *Journal of Materials Science*., **2018**, 53(1), p.716-726.

ELECTRIC PROPERTIES OF NI-C AND CO-C CORE-SHELL NANOPARTICLES IN POLYMER MATRIX

O. A. Syvolozhskyi[a], O. S. Yakovenko[a], L. Yu. Matzui[a], L. L. Vovchenko[a], V.V. Vilchinskyi[a], V.M. Bogatyrov[b]
[a] *Taras Shevchenko National University of Kyiv, Volodymyrs'ka Str., 64, Kyiv, 01601, Ukraine*
[b] *Chuiko Institute of Surface Chemistry, NAS of Ukraine, General Naumov Str., 17, Kyiv, 03164, Ukraine*
e-mail: mail.olexiy@gmail.com

Lots of metal-carbon nanostructured materials with metallic core/carbon shell nanoparticles were studied due to a wide range of applications in innovative areas of energy, biotechnology, etc [1, 2]. Among them systems with nickel core [1, 3] and cobalt core [2]. Such structures are presented as effective novel carbon adsorbents which work for the removal of organic contaminants [4].

The aim of this work was to investigate the electric properties on Ni-C and Co-C core-shell structures which are imbedded in polymer matrix. For investigations of transport properties bulk specimens from Ni-C and Co-C powder have been prepared by cold compacting with use of PVA (25 wt. %) as binder. The structure and morphology of the nanocomposites were characterized using SEM and XRD methods. It came out that filler particles of the composites consist of metal core coated with relatively uniform graphitic layers of several nanometers in thickness.



The dependence of electric resistivity of Ni-C core-shell structures in PVA matrix at $T = 77 \div 293$ K are presented in Fig. The results suggested that ρ_{293} / ρ_{77} is equal to 0.36 for the investigated nanocomposite.

[1] Anton, R. On the reaction kinetics of Ni with amorphous carbon, *Carbon*, **2008**, 46 (4), 656–662.

[2] Ramakrishnan, P. et al. Electrochemical performance of carbon nanorods with embedded cobalt metal nanoparticles as an electrode material for electrochemical capacitors, *Electrochim. Acta*, **2014**, 125, 232–240.

[3] Sterk, L. et al. Polymer-templated mesoporous carbons with nickel nanoparticles, *Colloids Surf. A*, **2010**, 362 (1–3), 20–27.

[4] Hayeeye, F. et al. Kinetics and thermodynamics of Rhodamine B adsorption by gelatin/activated carbon composite beads, *Colloids Surf. A*, **2017**, 513, 259–266.

MAGNETOTHERMOELECTRIC PROPERTIES OF BULK NANOSTRUCTURED SAMPLES OF $Bi_{85}Sb_{15}$ SOLID SOLUTION

Tagiyev M.M.[1,2]
[1]*Azerbaijan State Economic University (UNEC), Baku, Istiglaliyyat str., 6,*
[2] *Institute of Physics of the National Academy of Sciences of Azerbaijan, Baku,*
H. Javid ave., 131
e-mail: mail_tagiyev@mail.ru

Bi-Sb systems solid solutions, especially high-strength extruded materials based on them, are the most promising materials for creating various energy converters. Opportunities for increasing the thermoelectric efficiency of materials through the use of size effects, both classical and quantum, are currently being intensively investigated. In this sense, an approach based on the use of bulk nanostructured materials is interesting.

Bulk nanostructured samples of $Bi_{85}Sb_{15}$ solid solution were obtained using an AGO-2 ball mill. The average particle sizes in the powder were determined by means of XRD D8 ADVANCE X-ray apparatus, Bruker, Germany using the Scherrer formula.

In order to study the effect of nanosized particles on the thermo- and magnetothermoelectric properties of extruded $Bi_{85}Sb_{15}$ solid solution samples, their bulk nanostructured samples were obtained, consisting of particles with average sizes of $0.5 \cdot 10^5$, 380, 30 and 15 nm, and their electrical conductivity (σ) was studied, and the coefficients thermo-emf (α), Hall (R_H) and thermal conductivity (χ) in the temperature range ~80-300 K and magnetic field strength up to ~74×10^4 A/m. Samples that did not undergo post-extrusion annealing and the same samples that underwent annealing were studied. It was found that with decrease in the size of the powder in the extruded samples, an increase in the electrical conductivity σ and a decrease in the phonon conductivity (χ_{ph}) and thermoelectric coefficient α, Hall (R_H) coefficient is observed, i.e. dependences of these parameters of the samples on the size of the powders are satisfactorily correlated in all the studied temperature range. It is assumed that as the size of the crystals decreases, the concentration of boundaries increases, which leads to an increase in the concentration of electrons in the samples.

During extrusion due to plastic deformation in the samples, parallel to the formation of texture, structural defects are formed which are scattering centers for current carriers, which leads to a decrease in their mobility. The degree of texture during extrusion, the re-crystallization and disorientation of particles, the concentration of current carriers, the influence of a magnetic field on the electrical and thermal parameters of extruded samples of solid solutions also depend on the size of the particles in the sample.

ELECTRON TRANSPORT IN GRAPHENE: COMBINED EFFECTS OF STRAINS AND DEFECTS

Valentyn A. Tatarenko, Taras M. Radchenko
G. V. Kurdyumov Institute for Metal Physics of the N.A.S. of Ukraine, 03142 Kyiv, Ukraine
e-mails: tatar@imp.kiev.ua , tarad@imp.kiev.ua

As for all crystalline solids, the presence of a certain amount of disorder in graphene, — the thinnest known material nicknamed as a “miracle material” due to its superior electronic and mechanical properties, — is dictated by the second law of thermodynamics. Defects play a role of disorder and are always present in graphene samples due to the imperfection of the fabrication processes. Implementing the quantum-mechanical Kubo–Greenwood formalism for numerical calculation of dc conductivity, we demonstrate that the electron transport properties of graphene layer can be tailored through the combined effect of defects (point and line scatterers) and strains (uniaxial tension and shear). Defects and strains are commonly present in graphene due to the features of its growth procedure and when it is applied in devices. Being motivated by two experimental works [1, 2], where authors did not observe the transport gap even at large (22.5% of tensile and 16.7% of shear) deformations, we explain possible reasons with an accentuation on graphene’s strain and defect sensing. The revealed strain- and defect-caused electron–hole asymmetry and anisotropy of conductivity, its non-monotony as a function of deformation suggest perspectives for the strain–defect engineering of electronic and transport properties of graphene and related 2*D*-materials.

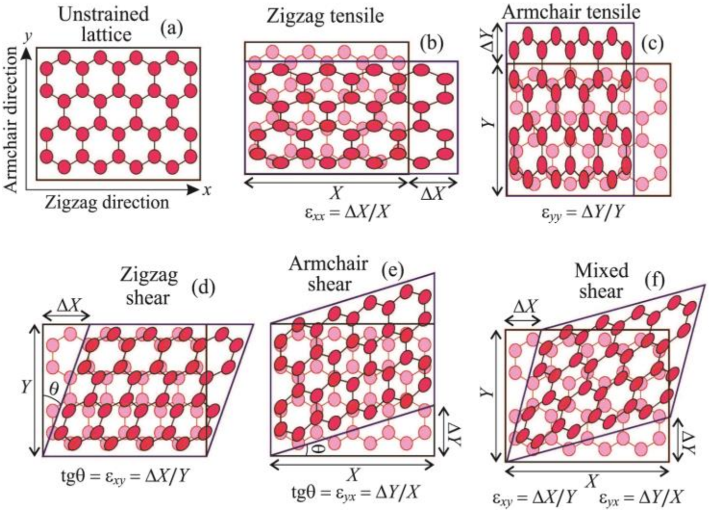


Fig. 1. Graphene lattice (a) deformed by different strains: zigzag- (b) or armchair-type (c) tensile deformation, shear strains along zigzag (d), armchair (e), or both directions (f), where ε_{xx}, ε_{yy}, ε_{xy}, and ε_{yx} are the strain tensor parameters.

[1] X. He, L. Gao, N. Tang et al., *Appl. Phys. Lett.* **104**, 243108 (2014).
[2] X. He, L. Gao, N. Tang et al., *Appl. Phys. Lett.* **105**, 083108 (2014).

THE TUNING OF ACID-BASE AND PROTON CONDUCTIVITY PROPERTIES OF THE TITANIA NANOSTRUCTURES BY CAREFULLY DOPING

G. Telbiz[a], N.Vlasenko[a], E.Leonenko[a], P. Smertenko[b], T Kavetskyy[c,d], P.Strizhak[a],
[a]L.V. Pisarzhevsky Institute of Physical Chemistry, Natl. Acad. of Sci. of Ukraine. Nauki av, 31, Kiev 03028, Ukraine
e-mail: gtelbiz@yahoo.com
[b, d]V.E. Lahskaryov Institute of Semiconductor Physics, Natl. Acad. of Sci. of Ukraine, Nauki av. 41, Kiev 03028, Ukraine
[c] Drohobych Ivan Franko State Pedagogical University, 82100 Drohobych, Ukraine
[d]The John Paul II Catholic University of Lublin, 20-950 Lublin, Poland.

Ability of the tuning of titania surface properties have gained a significant scientific interest and practical importance. For example, varied of the anion or cation doping concentration and conditions can be resulted in modification of the structure and surface chemistry of titania. Doping agents can be integrated into the titania lattice forming various surface defects and functional groups which significantly expands the possibilities of their practical application as effective photo and heterogeneous catalysts, sensor components, etc. In the present work, we show this possibility used new approach to sol-gel synthesis based on the using S- agents for doping of titanium oxide. The results of the integration of the doping elements in structures in situ of genesis of nanocomposites was received by used by a number of physical methods (XRD, XPS, FTIR, UV-VIS, TGA, TD MS, SEM, TEM, WAH, OETD, etc). The XRD and Raman data of the hydrothermally sol-gel synthesized titania nanostructures show that the anatase lattice strain became larger with increasing of doping agent. It was shown that using of sulfate ion during sol-gel synthesis result in the formation on the surface of anatase defects and functional groups that tuning of acidic-base properties of the surface of the composite. At an optimal concentration of the dopant, the composite structure has significant hydrophilicity, high density of interaction of OH groups on the surface and enhanced, relative to classical titania samples, electron, and proton conductivity on temperature range up to 250°C. The doping samples are characterized by a higher total acid capacity then the samples of pure titania and shows of the base properties for doping TiO_2 is especially higher, compared with pure titania.

dopingTiO2 is especially higher, compared with pure titania.surface and enhanced, relative to classical titania samples, electron, and proton conductivity on temperature range up to 250° C. The doping samples are characterized by a higher total acid capacity then the samples of pure titania and shows of the base properties for dopingTiO2 is especially higher, compared with pure titania.

IMPACT OF FILM MORPHOLOGY ON ELECTRONIC STRUCTURE IN THE PROTOTYPICAL SEMICONDUCTING POLYMER POLY-3-HEXYLTHIOPHENE

A. Vakhnin[a], A. Kadashchuk[a], A. Zhugayevych[b], A. Kohler[c]
[a] *Institute of Physics, National Academy of Sciences of Ukraine, 46 Nauki av., Kyiv 03028, Ukraine*
e-mail: vakhnin@iop.kiev.ua, kadash@iop.kiev.ua
[b] *Center for Electrochemical Energy Storage, Skolthech, Moscow, Russia*
[c] *Bayreuth Institute of Macromolecular Research (BIMF), University of Bayreuth, Bayreuth, Germany*

Semiconducting π-conjugated polymers are currently employed in organic solar cells and organic field-effect transistors mainly as they allow for a low-cost and low-temperature device fabrication compatible with flexible plastic substrates. It is commonly believed that charge transport in conjugated polymers is controlled by thermally activated hopping between segments of the same polymer chain separated from each other by topological defects and/or by carrier jumps between adjacent segments of different chains. The length of segments is subject to random variations that, together with random potential fluctuations caused by structural disorder, is the major source of the energy disorder in these polymers, implying a relatively broad density-of-states (DOS) energy distribution for neutral and charged excitations. The intrinsic energy disorder along with possible extrinsic traps are major factors limiting charge transport in these materials. Thus, an accurate picture of the density of states associated to traps and energetic disorder in such films is important as these have a strong impact on that aspect of the device performance which is related to charge carrier mobility.

Poly-3-hexylthiophene (P3HT) polymer is an archetypal organic semiconductor commonly used in different optoelectronic devices. Despite the P3HT is one of the most studied and technologically developed polymeric semiconductor, its structure-property relationships is still not fully understood. P3HT can adopt different morphologies and depending on solvent, temperature, molecular weight, and sample preparation, it can exist in an amorphous phase with coiled chain conformations or in an aggregated phase containing planarized chains prone to form semicrystalline domains. In this work we present a comprehensive spectroscopy and charge trapping studies using the low-temperature thermally stimulated luminescence technique in P3HT films of various polymorphs and morphologies. As a result, by combining several approaches we have resolved structure of semicrystalline P3HT and established new relationships between morphology and electronic properties.

SORPTION-LUMINESCENCE METHOD FOR DETERMINATION OF YTTERBIUM AND MORIN USING TRANSCARPATHIAN CLINOPTILOLITE

O. Stashkiv[a], V. Vasylechko[a,b], R. Gamernyk[a], G. Gryshchouk[a], A. Zelinskiy[a]
[a]*Ivan Franko National University of Lviv, 6 Kyryla and Mefodiya Str., 79005 Lviv, Ukraine;*
[b]*Lviv University of Trade and Economics, 9 Samchouk Str., 79011 Lviv, Ukraine*
e-mail: vasylechko@ukr.net

Ytterbium is widely used in electronics for the production of high-power fiber lasers, magnetic alloys, and also in nuclear power engineering. Morin belongs to the class of flavonoids that are derivatives of polyphenolic compounds. Flavonoids are effective natural antioxidants and have various phytotherapeutic effects. Morin, like other flavonoids, forms stable complexes with ions of lanthanides (Lns). Most of Lns and flavonoids are closely similar in their chemical properties. However, Lns essentially differ in their optical properties, in particular, in the ability for absorbtion and emission of excitation energy. Absorbtion of quantum light by Lns is accompanied by transition of electron in vicinity of 4f shell as well as between 4f and 5d states. The return transition of electron to corresponding sublevels of ground state causes the emission of light. This luminescence (LM) is specific for each Ln. In most cases, the methods of REEs and flavonoids determination require the samples pretreatment, which, in particular, includes preconcentration, separation and withdrawal them from natural objects, medicinal plants, technological solutions. For these purposes solid phase extraction and solid phase spectrofluorimetry using a variety of sorbents, including natural zeolites, are perspective. Transcarpathian clinoptilolite is an effective sorbent of trace amounts of Yb(III). It was found by X-ray fluorescence that using this natural nanomaterial it is possible to quantitatively separate Yb(III) from other REEs, in particular Pr(III), Nd(III), Eu(III), Ce(III), Sm(III), Sc(III) and Gd(III). Sorption of determined element on the solid matrix is one of the effective methods for increasing sensitivity and selectivity of LM determination. Natural zeolites have ability to include Ln ions in the grid using exchanged reactions. These ions save their ability to react with organic ligands. The sorbents that have been created on the zeolite surface have the ability to absorb UV – radiation and intensive LM. The possibility for determinations Yb and morin with using clinoptilolite as a sorbent was studied. The Yb(III)-clinoptilolite samples were obtained via lanthanide ions sorption from aqueous solution at pH 8.0 on the previously heated zeolite at 50°C in a solid phase extraction mode. The Yb(III)-clinoptilolite samples were dried at room temperature treated by the water-ethanol solution of morin at pH 8.0 in a static mode. For the excitation of LM samples rays with the wavelength of 365 nm were used. The intensity of the LM at 978 nm was chosen as analytical parameter for the quantitative determination of Yb and morin. The limit of detection of Yb(III) and morin is equal to 0.1 μg/mL and $3 \cdot 10^{-4}$M, respectively.

ENHANCEMENT OF RADIOLUMINESCENCE IN CERIUM DOPED MIXED OXYORTHOSILICATE NANOCRYSTALS $Lu_{2-x}Y_xSiO_5$:Ce^{3+}

V. Seminko, P. Maksimchuk, I. Bespalova, O. Viagin*, A. Aslanov, Yu. Malyukin
Institute for Scintillation Materials NAS of Ukraine, Nauky ave., Kharkiv, 61072, Ukraine
e-mail: viagin@isma.kharkov.ua

In the last decade, scintillation crystals of mixed cationic composition have been intensively studied. In a number of such crystals, an increase in the light yield is observed in comparison with unmixed crystals. There are several hypotheses explaining observed effect, including the modification of electron-phonon interaction, local fluctuations of the bandgap edges of the conduction and valence bands, and formation of clusters enriched by different cations.

In our studies, we have shown that such effect is also observed in nanocrystals. The nanocrystals of mixed lutetium-yttrium oxyorthosilicates $Lu_{2-x}Y_xSiO_5$:Ce^{3+} with Gd_2SiO_5-type structure were obtained. We have observed that the cation mixing in studied nanocrystals leads to sufficient increase of radioluminescence intensity as compared to Lu_2SiO_5:Ce^{3+} (in 2.5 times) which value is higher as compared to the one observed for corresponding bulk scintillation crystals. This effect cannot be explained only by redistribution of regular and irregular optical centers in nanocrystals. We believe that the observed increase of radioluminescence intensity can be interpreted as a combined effect of cation mixing leading to reduction of thermalization length of geminate electron-hole pairs and decrease of the content of electron traps formed by oxygen vacancies in mixed nanocrystals. The latter effect should be more pronounced for nanocrystals than for their bulk analogues due to higher content of oxygen vacancies in nanocrystals as compared to bulk crystals that can at least partially explain the stronger enhancement of radioluminescence intensity for mixed oxide nanocrystals.

INFLUENCE OF SILVER NANOPARTICLES ON PHOTOELECTROCHEMICAL CHARACTERISTICS of TiO_2-GO NANOCOMPOSITE

Sadykova A.E., Zhumabekov A.Zh., Ibrayev N.Kh.
Institute of molecular nanophotonics, Buketov Karaganda State University,
Universitetskaya Str. 28, Karaganda, 100026, Kazakhstan
e-mail: almar89-89@mail.ru

Graphene and its derivatives are currently being investigated for its application in many fields, such as photovoltaics, molecular electronics, etc. Nanocomposites based on TiO_2 and graphene oxide are attractive objects for use in photoelectrochemical and photocatalytic generation of hydrogen fuel and photocatalysis of organic pollutants. These properties can be improved by the phenomenon of localized plasmon resonance of metal nanoparticles (NP).

In this paper, we performed a study of the efficiency of electron transfer in the presence of Ag NP in semiconductor nanocomposite films based on graphene oxide (GO) and TiO_2. Their structural, photoelectrochemical, and photoelectric properties have been studied.

The nanocomposite material was synthesized using the hydrothermal method [1]. The concentration of GO was a wound of 5 wt%. Colloidal AG NP were synthesized by the method citrate reduction $AgNO_3$. The radius of the NP synthesized was 10 nm them were added to the nanocomposite at the stage of film preparation.

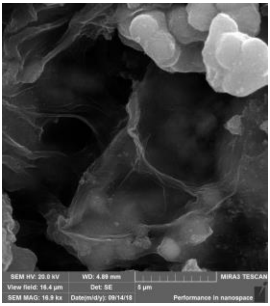


Fig.1. SEM image of the TiO_2/GO nanocomposite

Table 1 – Parameter values of the photocurrent in the TiO_2 films and the nanocomposites with different concentration of Ag NP

C_{Ag}, mole/L	I, µA	
	TiO_2	TiO_2–GO
0	20	65
10^{-13}	39	70
10^{-12}	42	101
10^{-11}	33	87

Measurements have shown that adding Ag NP to the nanocomposite increases its photocatalytic activity by almost 2 times (table 1). The increased photocurrent is the result of the interaction of silver NPs with TiO_2, which increases electron mobility, reduces the recombination of charge carriers, and allows additional injection of electrons directly from Ag NPs.

[1] Ibrayev N., Zhumabekov A., Ghyngazov S. and Lysenko E., *Materials Research Express*, **2019**, 6, 1-11.

ELECTRIC PROPERTIES OF GaSe <$NaNO_2$+PROPOLIS> NANOHYBRID ENCAPSULATE

Maksymych V.[a], Ivashchyshyn F.[a,b], Chabecki P.[b]
[a] *Lviv Polytechnic National University, Kotlyarevsky str, 1/1, Lviv, 79013, Ukraine*
e-mail: vitaliy.maksimich@gmail.com
[b] *Politechnika Częstochowska, Al. Armii Krajowej 17, Czestochowa, 42-200, Poland*

Non-organic/organic electronics is currently the most rapidly developing area of the research. A significant contribution is made by the development of supramolecular chemistry. It is caused by unlimited potential use of supramolecular compounds such as simple materials for electronics and complex biological systems.

An approach to creating complex non-organic/organic nanohybride structures with tailored properties is proposed in this paper. This approach is based on the phenomena and effects detected in clathrate assemblies with alternating semiconductor and organic nano-layers. Synthesized compounds were investigated with use of impedance spectroscopy and thermostimulated discharge methods.

Namely, the kointercalation of non-organic $NaNO_2$ and of organic molecules of propolis into the semiconductor Gallium Selenide gives rise to the effect of the frequency oscillations of the imaginary component of the complex impedance under the light. The synthesis of GaSe<$NaNO_2$+Propolis> reduces the loss tangent and leads to the increase in the dielectric constant. The value of the latter varies considerably in the magnetic field and light. This kointercalated guest component substantially changes electron and polarizable processes of the original matrices. At the same time, its volt-ampere characteristic (Fig. 1) clearly confirms its ability to accumulate electric energy from an external source of power. This effect is also called the memory effect.

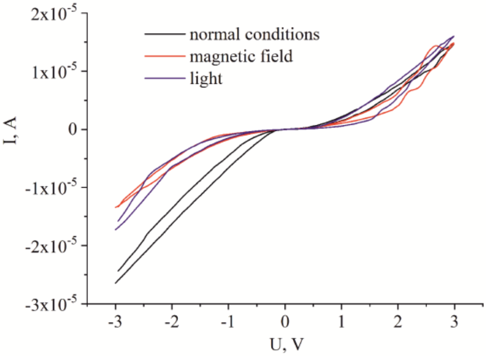


Fig. 1. Volt ampere characteristics GaSe<$NaNO_2$+Propolis >, measured in the normal conditions, in the magnetic field and in the illumination.

The paper presents a physical model to explain obtained results. These observed effects create the possibility to develop light controlled nano-structured reactive elements, photovaricaps with super capacity and nano-structured delay lines.

PLASMONIC NANOCAVITY METASURFACE BASED ON LASER-STRUCTURED SILVER SURFACE AND SILVER NANOPRISMS FOR THE ENHANCEMENT OF ADENOSINE NUCLEOTIDE PHOTOLUMINESCENCE

Anastasiia V. Tomchuk [a], Oleg A. Yeshchenko [a], Vladislav Yu. Kudrya [a], Igor M. Dmitruk [a,b], Nataliya I. Berezovska [a], Petro O. Teselko [a], Sergii Golovynskyi [c], Bin Xue [c], and Junle Qu [c]
[a] *Physics Department, Taras Shevchenko National University of Kyiv, 01601 Kyiv, Ukraine*
[b] *Department of Photon Processes, Institute of Physics, National Academy of Sciences of Ukraine, 03028 Kyiv, Ukraine*
[c] *Key Laboratory of Optoelectronic Devices and Systems of Ministry of Education and Guangdong Province, College of Physics and Optoelectronic Engineering, Shenzhen University, 518060 Shenzhen, China*
e-mail: nastiona30@gmail.com

A reliable photoluminescence (PL) spectroscopy and imaging of biomolecules at room temperature is a challenging and important problem of biophysics, biochemistry, and molecular genetics. [1] A unique effect of strong plasmonic enhancement of the PL by metal nanostructures is one of the most effective approaches for this purpose. [2] The highest enhancement is provided by metal nanostructures with densely packed sharp tips, periodically arranged metal nanostructures, and plasmonic cavities.[3,4] All of these features have been realized in the plasmonic cavity metasurface based on the silver (Ag) laser-induced periodic surface structure and Ag triangular nanoprisms studied in the present work. The strong plasmonenhanced PL of 5′-deoxyadenosine monophosphate deposited on such metasurfaces has been revealed at room temperature.

The observed enhancement of more than 1000-fold has been interpreted as a result of synergetic action of the generation of a high concentration of hot spots near the sharp edges of the laser-induced surface structure and nanoprisms together with excitation of the collective gap mode of the cavity due to strong near-field plasmonic coupling. Correspondingly, the plasmonic cavity metasurfaces consisting of metal laser-induced periodic surface structures and nonspherical metal nanoparticles with sharp edges have been shown to be crucial for the highly sensitive detection and imaging of biomolecules at room temperature without consuming any dye labels.

[1] Eastman, J.W.; Rosa, E.J., *Photochemistry and Photobiology*, **1968,** 7, 189.

[2] Li, A.; Isaacs, S.; Abdulhalim, I.; Li, S., *Journal of Phyical Chemistry C,* **2015**, 119, 19382.

[3] Xue, B.; Wang, D.; Zuo, J.; Kong, X.; Zhang, Y.; Liu, X.; Tu, L.;Chang, Y.; Li, C.; Wu, F.; Zeng, Q.; Zhao, H.; Zhao, H.; Zhang, H. *Nanoscale*, **2015**, 7, 8048.

[4] Hamad, S.; Podagatlapalli, G. K.; Mohiddon, M. A.; Soma, V.R., *Appied Physics Letters,* **2014**, 104, 263104.

SECTION 5

NONLINEAR PROPERTIES OF POLYMER COMPOSITES, NANOSTRUCTURES, NLO INFORMATION RECORDING

INFLUENCE OF ELECTROTHERMOPOLARIZATION ON PE+$PbCrO_4$ –BASED NANOCOMPOSITION STRUCTURES

M.A. Ramazanov[a], A.S. Huseynova[b], F.V. Hajiyeva [a], S.U. Atayeva[b]
[a]Baku State University, Baku
[b]Institute of Physics ANAS, Baku
e-mail: aem05@rambler.ru

Structural change of PE+$PbCrO_4$ nanocomposition by of method IR spectroscopy, AFM and photoluminescence spectra within wavelength λ=250-1000 nm have been studied. It is shown that photoluminescence spectra depend on the electrothermopolarization conditions. It is before electrothermopolarization at wavelengths 360nm, 374nm two maxima are observed. After electrothermopolarization two maxima are revealed at wavelengths 358nm; 373,07nm. The most intensive maximum of them is in the neighborhood of 358nm, the second is observed as the leg of the first one and arranged within 373,07nm. From Figures it is seen that photoluminescence spectra for PE+0,5%vol. $PbCrO_4$ nanocomposition change after electrothermopolarization, i.e. intensities of photoluminescence reduce sharply. Observed changes of spectra for nanocompositions are related to the changes of polymer supramolecular structure, degree of polymer interaction with the nanoparticle. Of IR spectrum is relatively ordinary, but after polarization in $PbCrO_4$nanophases there have been taken place structural changes, especially within frequency range 726 cm^{-1}, 732cm^{-1}, 825cm^{-1}. Before the polarization the oscillation intensities of CH_2 (726 cm^{-1}, 732 cm^{-1}, 825 cm^{-1}) in $PbCrO_4$ phase turned out to fall. However, after $PbCrO_4$ phase polarization the growth of CO oscillation peak intensities has been observed. The change in the frequency range owing to the polarization is related to the activation of CH valent oscillations in polyethylene. It is also seen that the band activation of CH valance, deformation oscillations as well interactions of CH_2 and CH group oscillations have been taken place. The appearance of extremely weak bands in intensity at 1528cm^{-1} up to 1625cm^{-1} in IR spectra is remarkable after polarization. Morphology of PE + $PbCrO_4$ nanocomposition has been investigated on scanning atomic force microscope. After electrothermopolarization $PbCrO_4$ nanoparticle increases the surface roughness, i.e. the surface non-homogeneity rises. As the histograms of the surface show before the electrothermopolarization $PbCrO_4$ nanoparticles are distributed over the wide range in sizes 250-450 nm. After electrothermopolarization the histograms of $PbCrO_4$ nanoparticle distribution surfaces in sizes 150-400 nm are narrow in behavior.

HIGH QUALITY PATTERNS PRODUCED BY NONLINEAR LASER LITHOGRAPHY FOR LIQUID CRYSTAL ALIGNMENT

Ihor Pavlov [a,b], Andriy Rybak [b], Andriy Dobrovolskiy [b], Zoya Kazantseva [c], Alpan Bek [a], Ozun Candemir [a], Ruslan Kravchuk [b], Igor Gvozdovskyy [b].

[a] *Department of Physics and Center for Solar Energy Research and Applications, Middle East Technical University, 06800 Ankara, Turkey*

[b] *Institute of Physics, NAS of Ukraine, 03028 Kyiv, Ukraine*

[c] *V.E. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine, 03028 Kyiv, Ukraine*

e-mail: ipavlov@metu.edu.tr

Mechanical rubbing and photo-alignment are the most widely used industrial technologies to create anisotropic surfaces for Liquid Crystal (LC) based devices. Recently, nonlinear laser lithography (NLL) was introduced as a fast, cost effective method for large area nano-grating fabrication [1]. Here we report on alignment of nematic LC on NLL treated Ti film deposited on glass for the first time. The setup (Fig.1 (a)) consists of a femtosecond fiber laser system, galvanometer-scanner and motorized 3D–translation stage. The samples were 300 nm Ti films deposited on glass. 5x5 mm^2 zones were created as shown on Fig. 1 (b, c). LC cells consisted of the tested and reference substrates where the last one was a glass substrate coated with a polyimide PI2555 and processed by the rubbing technique. The twist angle was measured by using the combined twist LC cell method, and the AAE was calculated from the obtained twist angles of different samples. We obtain controllable changes of the anchoring energy in the range between 2x10^{-6} J/m^2 to 10^{-4} J/m^2. Different macro-patterns based switchable phase masks were created which properties will be discussed.

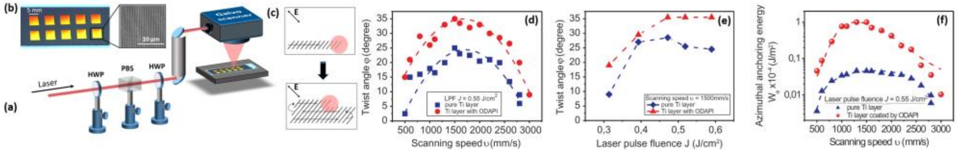


Fig. 1 (a) experimental setup, (b) example of the structured surface, (c) the mechanism of the structure formation, (d) dependence of the measured twist angle as a function of scanning speed at fixed pulse fluence 0.55 J/cm^2, (e) dependence of the measured twist angle as a function of pulse fluence at fixed scanning speed 1500mm/s, (f) dependence of the azimuthal anchoring energy as a function of scanning speed at fixed pulse fluence 0.55 J/cm^2. Blue lines – Ti surface processed by NLL, red lines – the same samples additionally coated by DMF solution of ODAPI.

[1] B. Öktem, I.Pavlov, S. Ilday, H. Kalaycıoğlu, A. Rybak, S. Yavaş, M. Erdoğan and F. Ö. Ilday, *Nat. Photon.* 2013, 7**,** 897.

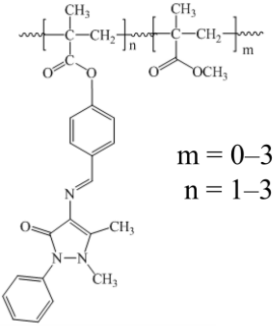
[2] I.Pavlov, A.Rybak, A.Dobrovolskiy, V.Kadan, I.Blonskiy, F.Ö.Ilday, Z.Kazantseva, I.Gvozdovskyy *J. Mol. Liq.* 2018, 212, 267.

We acknowledge *Scientific and Technological Research Council of Turkey* (TÜBİTAK) Project No 118F375

SYNTHESIS OF NOVEL POLYAZOMETHINE WITH ANTIPYRINE MOIETY: EFFECT OF COPOLYMER COMPOSITION VARIATION ON NONLINEAR OPTICAL RESPONSE

Valeriia Ovdenko[a], Volodymyr Multian[b], Dmitry Komarenko[b],
Oleksiy Kolendo[a], Volodymyr Gayvoronsky[b]
[a] *Taras Shevchenko National University of Kyiv, 60 Volodymyrska St., Kyiv 01033, Ukraine.*
e-mail: valeryovdenko@gmail.com
[b] *Institute of Physics, NAS of Ukraine, 46 Nauky pr., Kyiv 03028, Ukraine.*
e-mail: vlad@iop.kiev.ua

Polyazomethines belong to novel functional materials with promising chemical and optical properties, that can be applied in nonlinear optical and optoelectronic fields, including optical data storage, surface relief gratings, all optical switching, etc. In order to synthesize the polymers with an optimal combination of operational and given optical properties, a comprehensive investigation of copolymer composition effect on nonlinear optical (NLO) response should be done.



Homo- and copolymers containing 4-((1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-pyrazol-4-ylimino) methyl) phenyl moiety in the side chain were synthesized by the thermoinitiated free-radical polymerization process and characterized by FT-IR and ^{1}H NMR, techniques. The monomer reactivity ratios were estimated using Fineman-Ross (r_2 = 0.54) and calculation (r_2 =0.54±0.02) methods based on the data of original mole ratios of the monomers f_1 and the mole fractions of the monomer units in the copolymer.

The cubic NLO response of the films with thickness of about 1 μm was studied with self-action effects manifestation analysis of picosecond range laser pulses at 532 nm and 1064 nm [1]. In visible range a pronounced self-defocusing effect was observed with refractive NLO response efficiency $\mathrm{Re}(\chi^{(3)}) \sim -10^{-6}$ esu, being sensitive to the copolymer composition (n, m). The effect saturates at peak laser intensities ~ 200 MW/cm^2. In near IR range the films demonstrated dependent on polymer structure self-focusing or self-defocusing effects with reduced NLO response efficiency $|\mathrm{Re}(\chi^{(3)})| \sim 10^{-7}$ esu.

[1] V. Y. Gayvoronsky, A. Uklein, O. Kachkovsky, et.al., *Impact of Merocyanine Dye Concentration in Ultrathin Polymer Films on Nonlinear Optical Response Due to the Aggregation Effect*, *Mol. Cryst. Liq. Cryst.*, vol. 535, no. 1, pp. 132–139, 2011.

A DUAL-WAVELENGTH PULSED LASER PROCESSING PLATFORM FOR A-SI THIN FILM CRYSTALLIZATION

Volkan Türker[1], Mahmut Emre Yağcı[1], Sarper Haydar Salman[1], Kamil Çınar[2,3], Semih Koray Eken[1], Alpan Bek[2,3*]
[1] *FiberLAST Inc., METU Teknokent, Ankara 06800, Turkey*
[2] *Department of Physics, Middle East Technical University, Ankara 06800, Turkey*
[3] *The Center for Solar Energy Research and Applications (GÜNAM), Middle East Technical University, Ankara 06800, Turkey*
e-mail: volkanturker@fiberlast.com.tr , alpanbek@gmail.com

Interest in laser crystallization (LC) of silicon (Si) thin films has been on the rise in fabrication of polycrystalline silicon (pc-Si) based thin/ultrathin photovoltaic solar cells and Si based thin film transistors (TFT) [1,2,3,4]. Laser based fabrication of device quality pc-Si thin films at room temperature is expected to be a key enabling technology because of its low energy, material and process time budget. Fabrication of high-quality pc-Si thin films without pre-/post-treatment at large is a disruptive technology which has the potential to revolutionize the Si thin film industry [5,6]. We hereby describe in detail a multi-wavelength laser processing platform specially developed for crystallization of amorphous silicon (a-Si) thin films into pc-Si thin films. The platform has three main stages. The first stage consists of a nanosecond pulsed ytterbium (Yb^{3+}) doped fibre-laser with a master oscillator power amplifier architecture, operating at a wavelength of 1064 nm with an adjustable repetition rate between 80 kHz–300 kHz. The output beam has a maximum power of 18 W with a pulse energy of 90 µJ. The pulse durations can be set to values between 15 ns–40 ns. The second stage has free-space optical elements for second harmonic generation (SHG) which produces an emission at a wavelength of 532 nm. Conversion efficiency of the SHG is 25% with an output pulse energy of 20 µJ. The platform provides two wavelengths at either 1064 nm or 532 nm in crystallization of a-Si films for different crystallization regimes [2,7,8]. The last stage of the platform has a sample processing assembly with a line-focus, which has an x-y motorized stage on a vibration isolated table. Speed of the motorized stage can be set between 1 mm/s–100 mm/s. Stage speed and repetition rate adjustments help to adjust overlap of successive pulses between 97.22–99.99%. Our platform has variety of tune parameters that make it a uniquely flexible system for delicate Si thin film crystallization. A large selection of operational parameter combinations, the wavelength selection and simultaneous x-y scanning capability allow users to crystallize Si films on various substrates optimally. The operation wavelength choice can be done by considering optical absorption and thickness of a-Si films on different types of substrates. Hence, delivering precise amount of absorbed energy in the line-focus irradiation is useful in increasing the average size of crystalline domains; moreover, nucleation of crystallites can be initiated either from the top or bottom interface of the film.

Continuous and simultaneous motion of the stage in two dimensions allows to process arbitrary continuous pc-Si geometries in a-Si film. In summary, our multi-wavelength laser processing platform offers all-in-one LC utility for intricate LC-Si processing.

Keywords: laser; pulsed; second harmonic generation; crystallization; silicon; thin-film

[1] Çınar, K.; Karaman, M.; Bek, A. Improvement of laser-crystallized silicon film quality via intermediate dielectric layers on a glass substrate, *ACS Omega*, **2018**, 3, 5846–5852.

[2] Salman, H.S.; Bacıoğlu, A.; Eken, S.K. Crystallization of Hydrogenated Amorphous Silicon Thin Film on Glass by Using NS-Pulsed Fiber Laser Operating at 1064 nm, *Master’s Thesis, University of Hacettepe*, Ankara, Turkey, **2019**.

[3] Dore, J.; Evans, R.; Schubert, U.; Eggleston, B.D.; Ong, D.; Kim, K.; Huang, J.; Kunz, O.; Keevers, M.; Egan, R.; et al. Thin-film polycrystalline silicon solar cells formed by diode laser crystallization, *Prog. Photovolt. Res. Appl.*, **2013**, 21, 1377–1383.

[4] Sonntag, P.; Haschke, J.; Kuhnapfel, S.; Gabriel, O.; Amkreutz, D.; Rech, B. Properties of liquid phase crystallized interdigitated backcontact solar cells on glass, *Energy Procedia*, **2015**, 77, 487–492.

[5] Shah, A.; Torres, P.; Tscharner, R.; Wyrsch, N.; Keppner, H. Photovoltaic technology: The case for thin-film solar cells, *Science*, **1999**, 285, 692–698.

[6] Green, M.A. Third generation photovoltaics: Ultra-high conversion efficiency at low cost, *Prog. Photovolt. Res. Appl.*, **2001**, 9, 123–135.

[7] Jin, J.; Yuan, Z.; Huang, L.; Chen, S.; Shi, W.; Cao, Z.; Lou, Q. Laser crystallization of amorphous silicon thin films investigated by Raman spectroscopy and atomic force microscopy, *Appl. Surf. Sci.*, **2010**, 256, 3453–3458.

[8] Andra, G.; Bergmann, J.; Falk, F. Laser crystallized multicrystal-line silicon thin films on glass, *Thin Solid Films*, **2005**, 487, 77–80.

INFLUENCE OF SUBSTITUENTS ON PHOTORESPONSIVE BEHAVIOR OF METHACRYLIC POLYMERS CONTAINING 8-HYDROXY-QUINOLINE AZO-DYES IN SIDE-CHAIN

D. Chomicki[a], O. Kharchenko[b], A. Kozanecka-Szmigiel[c], D. Szmigiel[d], Ł. Skowroński[e],
J. Kowalonek[f], V. Smokal[b], O. Krupka[b], B. Derkowska-Zielinska[a]
[a]Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Torun, Grudziadzka 5, 87-100 Torun, Poland
[b] Faculty of Chemistry, Taras Shevchenko National University of Kyiv, Volodymyrska 60, 01033 Kyiv, Ukraine
[c]Faculty of Physics, Warsaw University of Technology, 75 Koszykowa Str., 00-662 Warsaw, Poland
[d]Sieć Badawcza Łukasiewicz – Instytut Technologii Elektronowej, Al. Lotnikow 32/46, 02-668 Warsaw, Poland
[e]Institute of Mathematics and Physics, UTP University of Science and Technology, S. Kaliskiego 7, 85-796 Bydgoszcz, Poland
[f]Faculty of Chemistry, Nicolas Copernicus University in Torun, Gagarina 7, 87-100 Torun, Poland
e-mail: chomicki@doktorant.umk.pl

In recent years, azobenzene-containing materials receive much scientific attention due to their optoelectronic properties, which make them attractive for such applications as optical data storage, optical switching, signal processing, nonlinear optical devices and many more. Azobenzene is constituted of two phenyl rings linked by an azo (–N=N–) bridge. It can appear in two isomeric forms (stable *trans* and metastable *cis*) with different spectroscopic properties and that makes reversible *trans-cis* photoisomerisation one of its important features [1]. When the azobenzene molecules embedded into polymer matrix are excited with linearly polarized light, after they go through multiple the *trans→cis→trans* cycles, they tend to align in such a way that the long axis of the molecule is perpendicular to the polarization direction. This allows to orient the molecules with light only and below the glass transition temperature of a polymer. As a consequence, birefringence and dichroism are induced in the material [2].

Spectroscopic properties as well as isomerisation quantum yields and thermal relaxation rate of azobenzenes can be tailored by introducing various electron donating/withdrawing substituents into the molecule and/or by the change in molecular structure. Understanding of a relationship between the structure and properties of azobenzene derivatives is crucial for designing materials suited for specific applications.

In this study we present optical properties of a novel class of methacrylic polymers containing 8-hydroxy-quinoline azo-dyes in side-chain. The goal of our study was to examine the influence of various substituents in the chromophores on the complex refractive index of the material and the ability to form surface relief gratings.

[1] B. Derkowska-Zielinska et. al, *Optical Materials*, **2018**, 85, 391-398.

[2] B. Derkowska-Zielinska et. al, *Journal of Physical Chemistry C*, **2020**, 124, 939-944.

SURFACE-INDUCED PHOTOREFRACTIVE EFFECT IN LIQUID CRYSTAL CELLS CONTAINING GOLD NANOPARTICLES

A. Gridyakina[a], H. Bordyuh[a], S. Bugaychuk[b], L. Viduta[b], V. Styopkin[b]
[a]*National Aviation University, Kosmonavta Komarova avenu 1, Kyiv 03058, Ukraine*
e-mail: gridyakina@nau.edu.ua
[b]*Institute of Physics of the NAS of Ukraine, Nauki avenu 46, Kyiv 03028, Ukraine*

Materials that exhibit nonlinear optical properties are of great interest for many contemporary applications, including manipulations of laser beams and optical information processing [1]. Liquid crystal (LC) materials are well known in practical applications due to their ability to change optical linear and nonlinear properties when an electric field is applied. The mechanism of nonlinear optical response in LCs is associated with reorientation of LC molecules in cell volume under the action of light. Pure nematic LCs exhibit surface-induced photorefractive effect. In this case, an inhomogeneous charge distribution on conductive (ITO) surface of substrate is induced by influence of light interference pattern on the LC cell. Created inhomogeneous electric field at the interface of LC molecules and ITO surface initiates reorientation of LC molecules. Reorientation of LC director starts from the interface and spreads over LC cell volume, creating modulation of a refractive index in the volume.

We have developed new type of hybrid LC cell, which contains gold nano-island film deposited onto ITO electrode. The absorption spectrum with a pronounced band in the visible range indicates surface plasmon resonance occurring in gold nanoparticles in the film. Cells exhibit nonlinear-optical response due to surface-induced photorefractive effect, where complex dynamics of unstable charge at inorganic-organic interface (ITO – gold island film – LC molecules) determines characteristics of this effect in hybrid LC cells.

We studied nonlinear optical characteristics in these cells varying the morphology of gold nano-island films, the value and type (dc, ac) of applied voltage, and the thickness of LC layer. For the studied cells we obtained large nonlinear optical coefficients as well as fast nonlinear optical response, which makes it possible to control the output intensities of beams using an alternating voltage of high frequency.

[1] S.Zwick, T.Gaist, M.Warber, W.Osten. Dynmic holography using pixelated light modulators, *Appl. Optics.*, **2010**, 49, is. 25, F47-F58.

[2] S.Bugaychuk, L.Viduta, L.Tarakhan, A.Gridyakina, H.Bordyuh, V.Cherepanov, A.Iljin, V.Nehytaylo. Optical linear and nonlnear properties of hybrid liquid crystal cells containing gold island films, *J.Mol.Cryst.Liq.Cryst.*, **2020**, accepted in publication.

NONLINEAR PROPERTIES OF MAGNETO-OPTIC DYNAMICS OF FERRONEMATIC LIQUID CRYSTALS

Korostil A.M., Krupa M.M.
Institute of Magnetism NASU and MESU, Vernasky str.,36b, 03142, Ukraine
e-mail: korostilandrii@gmail.com

Ferronematic liquid crystals (FNLC) represent novel type of the nematic liquid crystals in which the strong sensitivity of the molecular orientation to the external magnetic field is realized via the anchoring of ferromagnetic nanoparticle to the molecular ordering [1]. Corresponding change of optical anisotropy provides the low field and low consumption magneto-optic effect of the polarization twisting of the linearly polarized monochromatic beam transmitting through the NLC. These properties determine perspectives of utilizing such FNLCs for a variety of technological developments. Specially, it is light-driven modulators in optical schemes of the adaptive optics, electric and magnetic-controlled switches and attenuators of optical signals.

Main problems of FNLCs involve their structural stable with respect to ferromagnetic nanoparticle aggregation and speedup of magneto-optic dynamics together with the respond and relaxation under low field magnetic impact. Solving the first problem is related to the equilibrium between interparticle dispersion and magnetic attractive and repulsive Van-der-Waals interactions that are determined by the interphase interaction on the nanoparticle surfaces. The magneto-optic dynamics is determined by the energy functional of the FNLC and is described by the system of coupled equations for the molecular ordering parameter (so-called director) and ferromagnetic ordering parameter, magnetization, following from solving of the corresponding variation problem. In terms of the tensor operators [2] of molecular ordering, representing moments of spherical harmonics of different orders, it is obtained the self-consistent description of the magnetization and molecular ordering responses on the magnetic field impact.

[1] A. Mertelj, D. Lisjak, *Liquid crystals reviews*., **2017,** 5**,** 1-13.
[2] S. Mei, P. Zhang, *Multiscale Modeling. Simulation.*, 2015, **13,** 977-1000.

PLASMON SPECTRA AND OPTICAL CUBIC NONLINEARITY OF THREE-LAYER SRUCTURES: Au NANOPARTICLES - Al_2O_3 - PdO (Pd)

Brodin O.M., Brodyn M.S., Liakvovetskyi V.R., Rudenko V.I., Styopkin V.I
Institute of physics of NASU,46 Nauki ave., Kyiv 03028, Ukraine
e-mail: lyakh@iop.kiev.ua

A significant shift of the position of the surface plasmon resonance (SPR) of noble metal nanoparticles (NP) can be obtained by placing them on the surface of a conductive film. So the spectra and the nonlinear optical properties of such structures can be modified. Thus, the position of the SPR varied from the blue part of the spectrum to the IR band for silver NP on the gold surface separated by a layer of silicon oxide [1]. This shift was explained by the strong electromagnetic interaction of the NP and the metal film. The shift of SPR for gold NP on the graphene was observed in [2], and was explained by the charges transfer from gold NP to the graphene.

The authors of this work have created the three-layer structures: gold NP - palladium or palladium oxide film separated by an Al_2O_3 layer. However, the conductive films were placed not on the substrate, but covered NP. This significantly increased the optical stability of our samples under irradiation by laser pulses. The absorption spectra of the created structures were investigated and the SPR position dependence on the thickness of the Al_2O_3, PdO or Pd layers was determined.

The parameters of the nonlinear-optical response of these structures were measured by their irradiation with nanoseconds pulses of laser radiation $\lambda = 532$ and 1064 nm. The maximum value of the real part of the cubic nonlinear susceptibility Re $\chi^{(3)} = -7\times10^{-5}$ esu was obtained for the film Au = 5 nm, Al_2O_3 = 4 nm, PdO = 15 nm at a wavelength of 532 nm. This significantly high value makes such structures a promising material for applying it in optoelectronics devices. The mechanism of this nonlinearity is assumed. Under light irradiation free electrons in gold NP can heating, so can tunneling through a thin layer of isolator and reduce the polarizability of palladium oxide and give us a negative Re $\chi^{(3)}$, as we observed in our measurements.

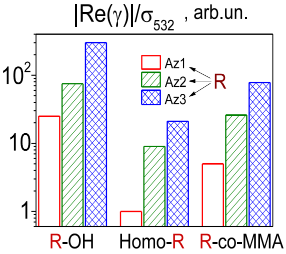
[1] M. Hu, A. Ghoshal, M. Marquez,| and P. G. Kik, *J. Phys. Chem. C*, **2010**, 114, pp. 7509–7514.

[2] H. Nan, Z. Chen, J. Jiang, J. Li, W. Zhao, Z.Ni, Xi.Gu and S. Xiao, *Phys.Chem.Chem.Phys.*, **2018**, 20, p. 25078.

SYNTHESIS AND NONLINEAR OPTICAL CHARACTERIZATION OF NOVEL AZO- AND AZOMETHINE CONTAINING POLYMERS WITH HETEROCYCLIC MOIETY

Valeriia M. Ovdenko[a], Volodymyr V. Multian[b], Andrii V. Uklein[b], Ihor V. Kulai[a],
Oleksiy Yu. Kolendo[a], Volodymyr Ya. Gayvoronsky[b]
[a] *Taras Shevchenko National University of Kyiv, 60 Volodymyrska St., Kyiv 01033, Ukraine.*
e-mail: valeryovdenko@gmail.com
[b] *Institute of Physics, NAS of Ukraine, 46 Nauky pr., Kyiv 03028, Ukraine.*
e-mail: vlad@iop.kiev.ua

Azo-containing dyes are one of the most popular materials in nonlinear optical (NLO) applications, used in optical data storage, surface-relief holography, optical switching, optical modulators and NLO devices. However, the incorporation of the photoactive moieties in the polymeric matrix can improve its operational characteristics. Therefore, polymers containing optically active chromophore groups with donor-acceptor substituted π-conjugated electron systems compound (D-π-A molecules) with azo- (-N=N-) or azomethine (-C=N-) π-bridges represent a promising class of nonlinear optical (NLO) polymers.



We have presented results of study of the refractive/absorptive nonlinear optical response efficiency tetrahydrofuran-based solutions of individual molecules and polymers via self-action effects manifestation of picosecond range laser pulses at 532 nm. A series of novel homo-/copolymers with heterocyclic antipyrine moiety have been synthesized by free radical polymerization. Polymer composition was controlled through the monomer feed ratio. Initial dyes, monomers and polymers structures were confirmed by FT-IR, ^{1}H NMR, and UV-Vis spectra. Special attention was paid to analyze effect (i) of chromophore structure (mono-/bis azomethine Az2/Az3), (ii) of type of π-bridges, and (iii) of number photoactive groups n_a on cubic hyperpolarizability γ of the studied materials.

All studied materials demonstrated efficient refractive NLO response with high magnitudes 10^2-10^3 of quality factor FOM. Efficiency of refractive NLO response per absorption cross-section at 532 nm $|\mathrm{Re}(\gamma)|/\sigma_{532}$ enhances from individual molecule through homopolymer to copolymer. The most promising results were obtained for copolymers of bent-shaped azomethine Az3-co-MMA.

[1] V. Y. Gayvoronsky, A. V. Uklein, O. D. Kachkovsky, *et al.*, *Effect of chromophore elongation on linear and nonlinear optical properties of merocyanines derivatives of diethylaminocoumarin*, J. of Mol. Struct., vol. 1045, pp. 191–198, 2013.

NONLINEAR LASER PROCESSING IN OPTICAL MATERIALS

S. Pavlova [a,b], V. Kadan [b], E. Yagci [a], K. Eken [a], I. Pavlov [a,b,c]
a. FiberLAST, A.S., Ankara 06531, Turkey
b. Institute of Physics of the NAS of Ukraine, Kyiv 03028, Ukraine
c. Department of Physics, Middle East Technical University, Ankara 06800, Turkey
e-mail: s.pavlov@fiberlast.com.tr , pasw@ukr.net

Nowadays c-Si and InP are one of the most widely used materials in electronic technology and sensor applications [1,2]. Despite the long-term use of these semiconductor materials and the high demand for optical-electronic integration, 3D laser processing technology inside of these materials is still a challenge. In transparent materials, the nonlinear absorption is strongly dependent on the laser intensity, as intense light readily causes ionization, which can be followed by a change in the lattice structure, and tight focusing is usually required to produce the modification. However, it is extremely difficult to achieve high values intensity inside these semiconductors due to the fast delocalization of the energy [3]. In our study, we demonstrate, the creation of optical waveguides and quasi-periodic structures deep inside c-Si (Fig. 1). The 3D modification was created by two types of lasers operating at 1550 nm: fs-laser (400 fs pulse duration, 2 μJ pulse energy at 250 kHz repetition rate) and ns-laser (5 ns pulse duration, 45 μJ pulse energy at 100 kHz repetition rate). The laser beam was focused inside c-Si and InP, and at some threshold values of energy in the volume of the crystal, the permanent modifications without changing the areas beyond the laser beam were observed.

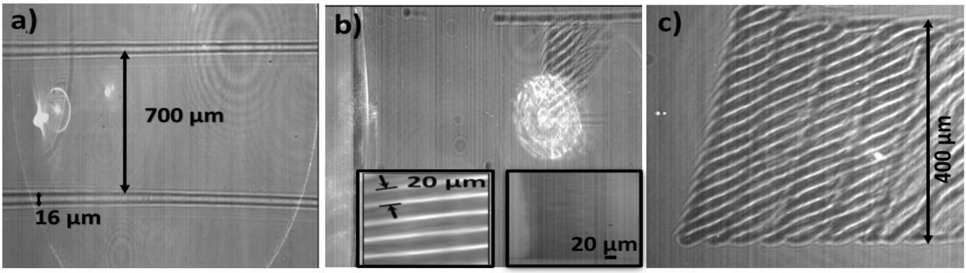


Fig. 1 The shadow images obtained in c-Si: a) the waveguides, (b,c) the periodic structure.

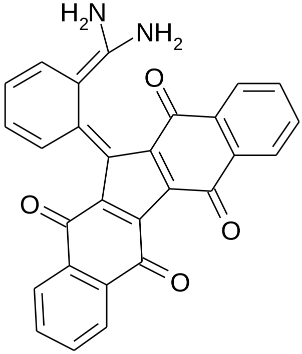
The formation of the periodic structures can be created anywhere inside the crystal (b,c). The insets in Fig.1 show the modifications created by fs (left) and ns (right) lasers. To summarize, we found that the morphology of subsurface modification depends on the laser pulse energy, scanning speed, repetition rate, and beam shape. Despite the difficulties, laser writing has the potential to make possible 3D structures in transparent semiconductors.

1. A. E.-J Lim et al., IEEE J. Sel. Top. Quantum Electron. 20, 405–416 (2014).
2. V. Zubyuk et al., ACS Photonics 6(11), (2019).
3. V. Kononenko, E. Zavedeev, V. Gololobov, Appl. Phys. A 122:293, (2016)

DIBENZOFLUORENE DERIVATIVE FOR NONLINEAR OPTICS AND SOLAR CELLS APPLICATIONS

A. El Haimeur[a,b], I. V. Levkov[b], T. V. Yegorova[b], A. I. Kysil[b], H. Bakkali[a], E. Blanco[a],
Z. V. Voitenko[b]
[a] *Department of Condensed Matter Physics and IMEYMAT: Institute of Research on Electron Microscopy and Materials, University of Cadiz, Campus Universitario de Puerto Real, E11510 Puerto Real, Cádiz, Spain*
[b] *Department of Organic Chemistry, Faculty of Chemistry, Taras Shevchenko National University of Kyiv, Volodymyrska Street, 64/13, Kyiv 01601, Ukraine*
z_voitenko@ukr.net

New organic materials become promising in the optoelectronic domains. The π-conjugated molecules guaranteed a high performance organic solar cells [1-3] because of their ideal spatial geometries in NLO applications, for example the benzene based compounds were improved for NLO applications, and a high performance inverted organic solar cells [1-3].



We report new one-step synthesized materials: the fluorene derivative with acceptor structure. New acceptor molecule with low ionization potential, and acceptor, has been designed, characterized and studied theoretically. The new material has been characterized by X Ray Diffraction, SEM and UV-Vis absorption. The results of the organic compounds revealed the fluorene derivative can be applied as light harvester candidates, in heterojunction solar cells and it can be applied in nonlinear optical device.

[1] M. Zhang, X. Zhan, *Advanced Energy Materials*, **2019**, 9, 1900860.
[2] L. Huo, J. Hou, S. Zhang, H. Y. Chen, Y. Yang, *Angewandte Chemie International Edition*, **2010**, 49, 1500.
[3] H. Shang, H. Fan, Y. Liu, W. Hu, Y. Li, X. Zhan, *Advanced Materials*, **2011**,23, 1554.

ANALYSIS OF THE FORMATION OF RELAXATION ZONES ON A SOLID SURFACE BY LASER NANOSTRUCTURING OF A MATERIAL

O.V. Yushchenko[a], O.S. Krivets[a]
[a] *Sumy State University, 2 Rimskii-Korsakov St., Sumy, 40007, Ukraine*
e-mail: o.yushchenko@phe.sumdu.edu.ua

Various methods of the formation of nanostructures on the surface of solids are of great interest to physical and chemical mechanics, metallurgy and solid state physics. Often, such structures occur during laser irradiation of the material and affect the physical properties of the material. In this regard, the development of the physical basis of new structuring methods, which lead to the formation of nanoscale reliefs on the surface of superhard ceramic materials, diamond films, metals and alloys, polymers and biomaterials, becomes relevant.

The impact on a solid of large mechanical loads caused by laser radiation is accompanied by residual deformation, the appearance of which is associated with the restructuring of the defective structure of the crystal. This can lead to an excited state of a macroscopically large number of crystal atoms. The relaxation of this excited state can occur due to the formation of new structure nuclei and relaxation zones [1]. Depending on the conditions of the external influence and deformation process, the relaxation zones can be groups of atoms or vacancies that form, for example, clusters, dislocation loops, micropores, as well as groups of dislocations or disclinations, microcracks, etc.

To analyze the behavior of the system, we chose the residual strain $\varepsilon_{ij}^{0}(r,t)$ as the order parameter and introduce the field of the relaxation process as $\varphi_{ik}(r,t) = \frac{1}{V_0}\int_{V_0} \varepsilon_{ij}^{0}(r,t)\,dV$. As a result, the system was presented by a self-consistent evolution of three values: the field of the relaxation process, the field of external stresses, and the concentration of relaxation zones. Using the proposed model, the attenuation of the relaxation process, the decay of the formed zones of relaxation, and the relaxation of stress were taken into account. Considering the effects of self-organization, the generation of the relaxation field due to the nucleation of relaxation zones was also taken into account using nonlinear relationships of the main parameters of the system. In addition, we investigated the conditions under which the processes of nanostructures formation on the surface during laser irradiation are realized by the first-order phase transition mechanism. The effective potential of the system was found analytically, potential minima correspond to the formation of stable states on the surface of the material. To confirm the results, a numerical calculation of the kinetics of the system was also carried out, and the corresponding phase portraits were constructed.

[1] V.Yu. Khomich, V.A. Shmakov, *Phys. Usp.*, **2015**, 58, 455–465.

SECTION 6

NOVEL MATERIALS, STRUCTURES, AND TECHNOLOGIES

POLYDOPAMINE AS AN EFFICIENT SORBENT FOR URANIUM EXTRACTION FROM NATURAL ENVIRONMENTS

V.N. Bliznyuk[a], K. Kołacińska[b], A.A. Pud[c], N.A. Ogurtsov[c], Y.V. Noskov[c], B.A. Powell[a], T.A.DeVol[a]
[a] *Environmental Engineering & Earth Sciences, Clemson University, Clemson, SC, USA*
[b] *Institute of Nuclear Chemistry and Technology in Warsaw, Poland*
[c] *V.P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry, NAS of Ukraine,*
50 Kharkivske shose, Kyiv 02160, Ukraine
e-mail: vblizny@clemson.edu

Interest to polydopamine (PDA) and PDA-based nanocomposites increased significantly due to the expanding range of existing and potential applications of this bioinspired polymer in energy storage, catalysis, filtration, biomedical systems, etc. [1]. PDA has a proven ability to remove/accumulate heavy metals/radionuclides from aqueous media. Amongst the many PDA applications, the environmental ones can be considered as very significant for remediation of industry, nuclear stations and waste disposal facilities, as well as of a possible recovery of radioactive elements from natural sources in groundwater or seawater. The latter is especially important because of ecological and possible commercial aspects (more than 99% of the world’s uranium stock is spread in the oceans) even despite the fact that natural concentration of U in the ocean is extremely low (~3.3 ppb).

In this presentation we will report on the retention properties and selectivity of PDA to uranium in natural aqueous environments. PDA polymer has been identified as a material with high sorption capacity for uranium at neutral pH (almost 500 mg/g) [2]. Its binding ability for uranium is realized probably due to formation of uranyl complexes with catechol- and amino- and other functional groups (Fig.1). This effect is synergistically enhanced especially at neutral pH by involvement of dimer or multimer forms of uranyl in the complexation process. The peculiarities of PDA-uranyl interaction responsible for the observed adsorption process were studied with a set of experimental techniques including FTIR spectroscopy, electron microscopy, X-ray photoelectron spectroscopy and cyclic voltammetry.

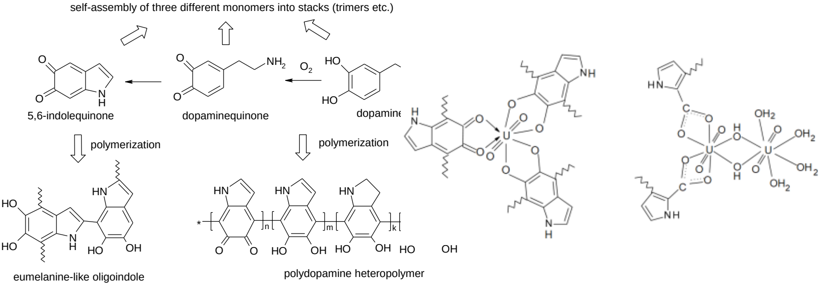


Fig.1 Alternative chemical structures of PDA (left) and formation of PDA-U complexes (right).

[1] H.Lee, S.M.Dellatore, W. M.Miller and P.B.Messersmith, *Science*, 2007**, 3180**, 426-430.

[2] V.N. Bliznyuk, K.Kołacińska, A.A.Pud, N.A.Ogurtsov, Y.V.Noskov, B.A.Powell, T.A.DeVol, *RSC Advances*, **2019**, 9, 30052-30063.

NON-DESTRUCTIVE DEPTH PROFILE RECONSTRUCTION OF INTERFACE BETWEEN BIOMOLECULES AND CARBON-BASED SURFACE USING ANGLE-RESOLVED XPS

Anna Artemenko[a], Oleg Babčenko[a], Egor Ukraintsev[a,b], Marian Marton[c], Marian Vojs[c], Tomas Wårgberg[d], Alexander Kromka[a]

[a]Institute of Physics of the Czech Academy of Sciences, Cukrovarnická 10, 16200 Prague 6, Czech Republic
[b]Faculty of Electrical Engineering, Czech Technical University in Prague, Technicka 2, 16627 Prague 6, Czech Republic
[c]Institute of Electronics and Photonics, Slovak University of Technology, Ilkovičova 3, SK-812 19 Bratislava, Slovakia
[d]Department of Physics, Umeå University, Linnaeus väg 24, Umeå 90187, Sweden
e-mail: artemenko@fzu.cz

Carbon-based materials (diamond, diamond-like carbon (DLC), graphene, etc) are known as a promising platform for the development of highly tunable biomolecular interfaces. However, it is a challenge to make a proper modification of carbon-based surfaces and control the adhesion of biomolecules on them. Obviously, an understanding of actual mechanisms of interactions of biomolecules with carbon-based surfaces requires advanced surface analysis of the interface between organic/inorganic material.

Here we report on investigations of the interaction of biomolecules (amino acids) with H-, O-functionalized atomically-flat monocrystalline diamond (MCD), nanocrystalline diamond (NCD) and DLC films using X-ray photoelectron spectroscopy (XPS). The depth distribution (<10 nm) of bonding states was calculated from the angular-resolved XPS spectra using the maximum entropy method (MEM), i.e. the in-depth reconstructions of the bonding states at the interface between carbon-based materials and biomolecules. The in-depth distributions of the resolved bonding states revealed the dependence of C-N bonds from biomolecules on the surface termination of carbon-based materials.

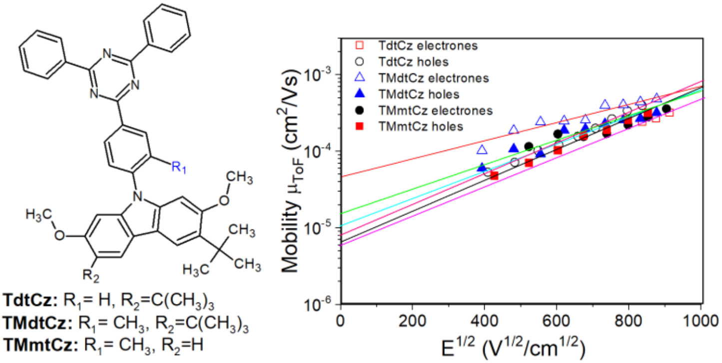
The XPS analysis was accompanied by other comprehensive methods like AFM, SEM and WCA. For instance, AFM measurements revealed differences in the thickness of the adsorbed biomolecular layer on NCD and DLC films depending on surface termination. The correlation between the obtained results will be discussed.

The work is supported by Operational Programme Research, Development and Education financed by European Structural and Investment Funds and the Czech Ministry of Education, Youth and Sports (Project No. CZ.02.2.69/0.0/0.0/18_053/0016627) and by project VEGA 1/0554/20 and by the Czech Science Foundation (project No. 20-00925Y).

2,7-DIMETHOXYCARBAZOLE AND TRIAZINE BASED BIPOLAR MATERIALS FOR OLEDs: SYNTHESIS AND INVESTIGATION

A. Bucinskas[a], A. Gruodyte[a], O. Bezvikonnyi[a], D. Volyniuk[a], J. V. Grazulevicius[a]
[a]*Department of Polymer Chemistry and Technology, Kaunas University of Technology,*
Radvilenu St. 19, LT-50254, Kaunas, Lithuania
e-mail: audrius.bucinskas@ktu.lt

The widely used strategy to achieve bipolar materials is to incorporate electron-donating and electron-withdrawing (D-A) moieties into the same molecule, facilitating injection and transport of both holes and electrons.[1,2] Moreover, to achieve higher efficiency of OLEDs the balanced hole and electron transport for efficient exciton recombination in emission layer is obligatory. Taking into account these considerations, a series of 2,7-dimethoxycarbazole and triazine derivatives was designed and synthesized. New compounds exhibited balanced charge transporting properties (Figure 1).



TdtCz: R_1= H, R_2=$C(CH_3)_3$
TMdtCz: R_1= CH_3, R_2=$C(CH_3)_3$
TMmtCz: R_1= CH_3, R_2=H

Figure 1. Hole and electron mobilities versus electric field.

The main aspects of the synthesis, characterization (photophysical, optical, thermal, electrochemical, charge transporting properties) and time-dependent density functional theory (TD-DFT) calculations will be reported in the presentation.

References
[1] S. Hu *et.al. ACS Appl. Mater. Interfaces*. **2019**, 11, 27134–27144.
[2] M. Godumala, *et.al. J. Mater. Chem. C*. **2019**, 7, 13930–13938.

This work was supported by the Research Council of Lithuania (Grant No S-LU-20-12).

STIMULATED EMISSION OF MEROCYANINE DYE IN POROUS ALUMINIUM OXIDE MATRIX

D.A. Afanasyev[a], N.Kh. Ibrayev[a], A.A. Ishchenko[b],
[a] *Institute of Molecular Nanophotonics, Buketov Karaganda State University, Universitetskaya 28, 100028, Karaganda, Kazakhstan*
[b] *Institute of Organic Chemistry, National Academy of Sciences of Ukraine, Murmanskaya 5, 02094, Kiev, Ukraine*
e-mail: a.d.afanasyev2@gmail.com

Properties of a merocyanine dye (MD) stimulated emission (SE) in thin film of a porous aluminium oxide (PAO) were investigated for the first time. PAO thin films were obtained by electrochemical anodization in an electrolyte based on sulfuric acid. The pore diameter was ~ 15-20 nm.

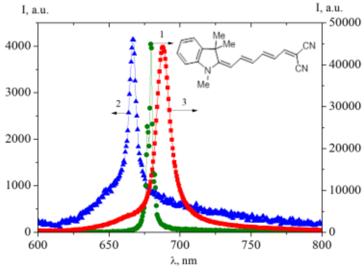


Fig. 1. Spectra of SE for MD: 1 - in ethanol C = 2.5 · 10^{-4} mol, P = 5.2 MW/cm^2; 2 - POA film, P = 160 MW/cm^2; 3 - POA film with PMMA, P = 40 MW/cm^2

Absorption and fluorescence spectra of the dye in PAO film were measured. Maximum optical density (*D*) of the dye molecules in POA is at 620 nm, and fluorescence at 650 nm. The lifetime of the dye fluorescence in the films is 0.98 ns, higher than the lifetime in ethanol τ_f = 0.37 ns. Quantum yield (Φ_f) of MD fluorescence in the solution was Φ_f= 0.061 at C = 10^{-6} mol/L, in the PAO film was Φ_f = 0.003.

Spectra of SE of the dye were shown in fig. 1. Properties of SE of the dye in ethanol were researcher in detail in [1]. SE of MD in the films occurs at high values of a pump power density (> 100 MW/cm^2). Lasing threshold is *Ptr* = 103 MW/cm^2. Low effective dye generation may be cis-trans photoisomerization of the dye molecules, as well as the interaction of the dye with molecular oxygen [2]. Polymethylmethacrylate (PMMA) film was deposited on the surface of POA for the protect MD from external influences. The lasing spectrum in PAO film with PMMA is shown in Fig. 1, curve 3. Adding a polymer leaded to a shift in the maximum of SE to 687 nm and a decrease in the value *Ptr*= 3 MW/cm^2. The Q-quality has close values for the films before applying PMMA and after its application (*Q*≈57).

[1] Butrimovich O.V., Voropay E.S., Ksenofontova N.M., Samtsov M.P. *All-Union Conference: Inverse population and generation at transitions in atoms and molecules.* Tomsk, **1986**. 52.

[2] Afanasyev D.A., Ibrayev N.Kh., Omarova G.S., Kulinich A.V., Ischenko A.A. *Optics and Spectroscopy*, **2020**, 1, 61.

IR-FOURIER TRANSFORM SPECTROSCOPIC STUDY OF SYSTEMS NaNO-Al_2O_3 + NaNO-SiO_2 + H_2O

[1]Agayev T.N., [1]Melikova S.Z., [2,3]Tagiyev M.M.,
[2]Dzhafarova S.Z., [2]Akhmedova A.M.
[1]Institute of Radiation Problems of NAS of Azerbaijan, Baku, B. Vahabzadeh str., 9
[2]Azerbaijan State Economic University (UNEC), Baku, Istiglaliyyat str., 6,
[3] Institute of Physics of the National Academy of Sciences of Azerbaijan, Baku, H. Javid ave., 131
e-mail: agayevteymur@rambler.ru

Nanosized oxide compounds of aluminum and zirconium are widely used as active components and an effective catalyst carrier for various processes, including in radiation-catalytic processes for the production of hydrogen from water. This work presents the results of IR-Fourier spectroscopic studies of radiation decomposition of water in a heterogeneous system of nano-Al_2O_3 + nano-SiO_2 + H_2O at room temperature ($T = 300$ K) under the influence of γ-quanta in order to establish the role of intermediate-active particles (radical groups) in these processes. The ratio of nano-Al_2O_3 + nano-SiO_2 nanopowders varied: 50% nano-Al_2O_3 + 50% nano-SiO_2, 22, 22% nano-Al_2O_3 + 77, 28% nano-SiO_2 and 22,22% nano-SiO_2 + 77, 28% nano-Al_2O_3. IR Fourier absorption spectra were recorded on a Varian 640FT-IR spectrometer in the range 4000–400 cm^{-1} at room temperature. For this, tablets 50–100 μm thick were pressed from Al_2O_3 and SiO_2 nanopowders. The IR spectra of the samples were measured in a special quartz cuvette with CaF_2 windows, which allows one to obtain the spectra of adsorbed water decomposed under the influence of γ-radiation. In the IR spectrum, in the region of lattice vibrations in dehydrated n-Al_2O_3 samples, a wide band of 900–850 cm^{-1} appears, which is characteristic of the Al_{14} – O bond, where aluminum cations are in tetrahedral coordination. The absorption bands at 330, 370, 480, 620, and 735 cm^{-1} are related to the octahedral position of the aluminum cation. In the region of lattice vibrations of nano-SiO_2 (1400–400 cm^{-1}), absorbance bonds (AB) with maxima of 472, 798, and 1095 cm^{-1} are detected in the spectra, which are related to symmetric and asymmetric stretching vibrations of Si – O and Si – O_2 – Si. A change in the ratio of Al_2O_3 and SiO_2 nanopowders is accompanied by a redistribution of the Al – O and Si – O AB intensities. In an unirradiated heterosystem, after water adsorption on the surface of aluminum and silicon dioxide in the region of stretching vibrations of OH groups, AB appear that indicate the occurrence of molecular form adsorption. Thus, the possibility of applying the method of infrared Fourier spectroscopy to study radiation processes in the heterogeneous system of nano-Al_2O_3 + nano-SiO_2 + H_2O at room temperature under the influence of γ-quanta has been shown. It was revealed that water adsorption in aluminum and silicon nanooxides proceeds by molecular and dissociative mechanisms.

The laws of radiation-stimulated adsorption and radiation-catalytic conversion of water in the presence of aluminum and silicon nanooxides obtained on the basis of IR spectroscopic spectra can be used to develop the scientific basis for the selection of effective catalysts for radiation technology.

NOVEL HYBRID TITANIUM-CONTAINING INTERPENETRATING POLYMER NETWORKS WITH EFFICIENT UV-INDUCED CHARGES SEPARATION

Tetiana T. Alekseeva , Nataly V. Kozak, Nataly V. Iarova
Institute of Macromolecular Chemistry of the National Academy of Science of Ukraine,
Kharkiv highway, 48, Kyiv 02160, Ukraine
e-mail: tatianalekseeva49@gmail.com

Titanium-containing interpenetrating polymer networks (Ti-IPNs) based on the cross-linked polyurethane (PU), poly (hydroxyethyl methacrylate) (PHEMA) and poly (titanium oxide) ($(–TiO_2–)_n$), previously synthesized by sol-gel method in the presence of 2-hydroxyethyl methacrylate **(**HEMA) were obtained. The formation of $(–TiO_2–)_n$ occurred by hydrolysis-condensation reactions of $Ti(OPr^i)_4$, in the presence of 0.1 N HCl as the catalyst. The molar ratio of HEMA/$Ti(OPr^i)_4$ was 8/1 and the molar ratio of Ti $(OPr^i)_4/H_2O$ were 1/1 (sample Ti-IPN-1) and 1/2 (sample Ti-IPN-2). The ratio of PU/PHEMA components in the IPN and Ti-IPNs was 30/70 wt %.

The DSC studies of Ti-IPN have shown that the obtained polymer systems, as well as the initial IPN, have a two-phase structure, as evidenced by the presence of two heat capacity jumps (ΔC_p) on the temperature dependence of $C_p = f(T)$. The introduction of poly (titanium oxide) in the initial IPN increases the glass transition temperature of the PU phase, but the glass transition temperature of the PHEMA phase is practically unchanged. Contrast to dynamical mechanical analysis (DMA) the DSC method allows the identification of PU phase formation in polymeric Ti-IPNs systems.

The results obtained by method of optical spectrophotometry have shown that the light transmission coefficients (T, %) of Ti-IPNs samples before UV-irradiation evaluated at λ=650 nm was (90.7-91.0) %. The optical transparency for Ti-IPNs samples after UV-irradiation within 240 minutes decreased to 61.0% (Ti-IPN-1) and 48.0% (Ti-IPN-2), respectively. The Ti-IPN samples UV-irradiated area became black. The differences observed are apparently due to the different morphology of poly (titanium oxide) in Ti-IPN-1 and Ti-IPN-2 hybrids, which affects the efficiency of the formation of Ti^{3+} centers.

According to EPR data UV irradiation on air at room temperature of samples of Ti-IPNs is accompanied by the appearance of signal of paramagnetic centers with broad isotropic signal at $\mathbf{g_1}$= 2.010 and also noticeably split signal at $\mathbf{g_2}$ = 2.003 and $\mathbf{g_3}$ =1.967. First and second of them can be ascribed to oxygen contained “hole scavenger” were as the third one to Ti^{3+}paramagnetic ions.

Such a signal is not present in the initial sample spectrum. The low rate of the electron–hole pair recombination in Ti-IPN matrix at 25°C demonstrates efficient separation of the charged particles in a hybrid material and can be approximated by the inverse function $y= 1/(a+b/t)$. Using nitroxyl spin probe it was revealed essential compaction of the polymer matrix (twofold Ti-IPN-1 and three times Ti-IPN-2) due to irradiation-recombination processes.

ELECTRON AND HEAT TRANSPORT IN SnTe CRYSTALS WITH VARIOUS VACANCY CONCENTRATIONS IN TIN LATTICE

T.D. Aliyeva, G.Z. Bagiyeva, N.M. Akhundova*, G.D. Abdinova, B.Sh. Barkhalov

Institute of Physics of the National Academy of Sciences of Azerbaijan,
AZ 1143, Baku, H. Javid ave., 131
e-mail: tunzalaaliyeva@mail.ru
** Azerbaijan State Economic University (UNEC)*,*
AZ 1001, Baku, Istiglaliyyat str. 6

The promising medium-temperature thermoelectric material SnTe has a complex valence band, crystallizes with a deviation from stoichiometry, and its samples contain electrically active vacancies in the tin sublattice with a concentration of up to 10^{20} cm^{-3}. This leads to a number of features in the transport properties (electrical and thermal) of crystals of this compound, the mechanisms of which are not fully understood, which limits the use of this material and its solid solutions. Structural vacancies, as scattering centers for electrons and phonons, should also manifest themselves during electron and heat transfer in SnTe samples. In this regard, the preparation of SnTe crystals with various concentrations of vacancies in the tin sublattice and the study of their electrical and thermal properties are of certain scientific and practical importance. It can be assumed that the concentration of vacancies in SnTe crystals in the tin sublattice can be reduced by introducing superstoichiometric excess Sn atoms into the crystal. This will make it possible to obtain SnTe samples with various concentrations of vacancies and study the role of structural vacancies in the tin sublattice in the process of transfer of electric charge and heat.

For this purpose, in the present work by the Bridgman method were obtained SnTe single crystals with excess (super-stoichiometrically introduced) tin atoms up to ~1.0 at.% and studied their electrical conductivity σ, thermoelectric coefficient α and thermal conductivity χ in the range of 90-300 K.

Based on the measured values of σ, α, χ, the electronic χ_e and lattice χ_l parts of thermal conductivity, thermal resistance created by structural defects (mainly, by vacancies in the tin sublattice) are calculated. It was shown that the temperature dependences of σ an α of the samples are satisfactorily explained by the model of two valence bands of SnTe, and of thermal conductivity - by phonon-phonon scattering. Excessively introduced Sn atoms up to 0.05 at.%, being distributed over the crystal, create donor centers scattering phonons and compensating doubly charged vacancies in the tin sublattice, which leads to a decrease in χ_l, χ_e and σ. Above 0.05 at.%, excess atoms, filling these vacancies and creating additional impurity centers, increase χ_l, χ_e and σ.

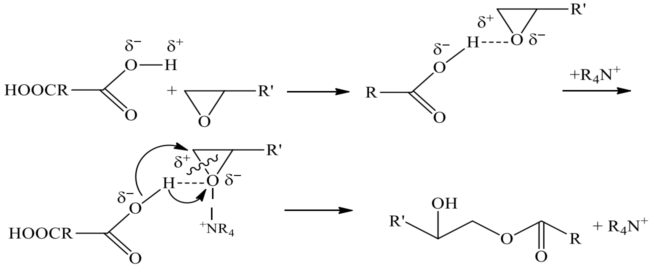
The electrical and strength properties of alloyed ohmic contacts of SnTe single crystals with different contents of excess tin atom with eutectic mass % 57Bi + 43Sn were also investigated. It was found that the contacts are contacts are quite low-resistance and durable, and the flow of current through them occurs mainly along the metal shunts formed in the process of creating a contact.

THE MECHANISM OF EPOXY COMPOUND AND ADIPIC ACID REACTION

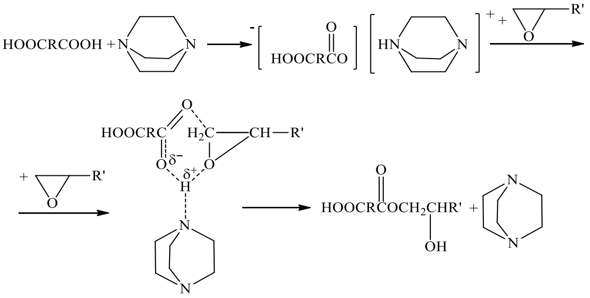
Olena Astakhova, Olena Shyshchak, Michael Bratychak
Lviv Polytechnic National University, 12 Bandery St., Lviv 79013, Ukraine
e-mail: mbratychak@gmail.com

When epoxides are modified with dibasic acids of aliphatic and aromatic types, the products with free epoxy and carboxy groups are obtained. Among the catalysts proposed for the reaction between epoxide oligomer and dibasic acid are benzyltriethylammonium chloride (BTEACh) or 1,4-diazobicyclo[2,2,2]octane (DABCO). But the reaction mechanism is not described. So the aim of our work was to propose such mechanism.

It was established that in the presence of BTEACh, in isopropyl alcohol medium, the reaction between dibasic carboxylic acid and the epoxide occurs *via* the formation of the complex



When using DABCO as a catalyst, the reaction mechanism takes a view:



Thus, in the presence of BTEACh as a catalyst, the most probable is the formation of the final product due to the electrophilic cation $^{+}NR_4$ attack on epoxide by oxygen atom. DABCO, as the catalyst, and adipic acid form salt, which further forms an intermediate six-member transition complex in the presence of an epoxide. During complex decomposition the catalyst is released and the resulted oligoester is formed.

THERMODYNAMIC FUNCTIONS OF PHASE TRANSITIONS OF COMPOUNDS A_8GeX_6 (A=Ag, Cu; X=S, Se)

[a]Bayramova U.R., [a]Mashadiyeva L.F., [b]Shukurova G.M., [a,b]Babanly M.B.
[a]*Institute of Catalysis and Inorganic Chemistry, ANAS,113, H.Javid, AZ-1143, Azerbaijan*
[b]*Baku State University, Z.Khalilov str., 23, AZ-1148, Azerbaijan*
e-mail: babanlymb@gmail.com

The argyrodite family compounds with the general formula $A_8B^{IV}X_6$ (where A - Cu, Ag; B^{IV} - Si, Ge, Sn; X - S, Se, Te) possess a number of valuable functional properties and are the subject of investigation by many research groups. A number of representatives of this class have mixed ion-electron conductivity, which makes them very promising for use in the development of photoelectrode materials, electrochemical converters of solar energy, ion-selective sensors, etc. [1-3]. Most of these compounds have phase transitions at relatively low temperatures (40-250 °C). The thermodynamic properties of phase transitions of these compounds have not been studied.

The aim of this work was to determine the thermodynamic functions of phase transitions of A_8GeX_6 compounds by the DSC method.

For research, the ternary compounds Ag_8GeS_6, Ag_8GeSe_6, Cu_8GeS_6 and Cu_8GeSe_6 were synthesized by direct fusion of stoichiometric amounts of the corresponding elementary components of high purity (99.999%) under vacuum in a two-zone mode. Then, the samples were annealed at 500 °C (100 h) and at a temperature below the phase transition temperature of these compounds (10 h). The synthesized compounds were identified by DTA and XRD. The temperature and heats of phase transitions of Ag_8GeS_6, Ag_8GeSe_6, Cu_8GeS_6 and Cu_8GeSe_6 compounds were determined by DSC. The studies were performed on a Linseis DSC400 differential scanning calorimeter, and the results were evaluated using the *Linseis TA Evaluation V 2.3.1* software. From the values of the molar enthalpy of phase transitions, the molar entropies of these transitions were calculated. It was found that the entropies of phase transitions of the studied compounds have abnormally high values, which is probably due to the delocalization of silver and copper cations upon transition to a high-temperature ion-conducting cubic modification.

This work was supported by the Science Development Foundation under the President of the Republic of Azerbaijan – Grant № EİF-BGM-4-RFTF-1/2017-21/11/4-M-12

[1] Babanly M.B., Yusibov Y.A., Abishev V.T. *Ternary chalcogenides based on copper and silver*. Baku: BSU, 1993, 342 p. (In Russian).
[2] Li L., Liu Y., et al., *J. Mater. Chem. C*., **2016,** 4, 5806.
[3] Jiang B., Qiu P., et al. *Journal of Materials Chemistry C*, **2017**, 5(4), 943–952.

ACRYLIC ACID MODIFIED LDH FOR NANOSTRUCTURED POLYMER MATERIALS

I. Bei[a], V. Budzinska[a], O. Slisenko[a], O. Tolstov, N. Iukhymenko[b]
[a] *Institute of Macromolecular Chemistry NASU,*
48, Kharkivske shose str., Kyiv 02160, Ukraine
e-mail: irynabei@meta.ua
[b] *Taras Shevchenko National University of Kyiv,*
60, Volodymyrs'ka str., Kyiv 01601, Ukraine

Synthetic layered double hydroxides (LDH) are promising materials for using in different applications such as catalysis, waste water treatment, electrochemical sensors, drug/gene delivery systems. One of the most important area of their application are polymer/LDH nanocomposites due to the extraordinary improvements in mechanical and thermal properties, reduced gas permeability and flame retardancy compared to neat polymer and conventional organic-inorganic composites. The main challenges of polymer/layered inorganic nanocomposites preparation are exfoliation of filler stacks and homogeneous dispersion of 2-dimensional inorganic platelets in polymer matrix. Using LDH this problem could be solved by appropriate choice of both cationic composition of LDH lamella and type of interlayer negative counterions. Introduction of organic anions into LDH interlayer space provides increased affinity of inorganic filler to polymer matrix. It can be assumed that chemical interaction between LDH counterions and polymer's functional groups promote better compatibility of composites constituents. Using substances with both anion and double bond functionalities followed by *in situ* polymerization seems to be the most promising approach in polymer/LDH nanocomposites preparation.

In this work Zn/Al LDHs containing interlayer acrylic acid anions were synthesized. Three common methods of organic anions introduction into interlayer space were used such as ion exchange process, *in situ* modification as well as reconstruction method and their efficiency were compared. The structure of LDHs obtained was controlled by X-ray diffraction and the presence of acrylic acid anions in the interlayer space was confirmed by IR spectroscopy. Moreover, redox titration method was adapted to determine the concentration of acrylic acid anions intercalated into LDH.

Effect of acrylic acid modification of LDH on polymerization of 2-hydroxyethyl methacrylate (HEMA) as well as structure and properties of the prepared poly(HEMA)/LDH nanocomposites was studied and discussed.

PULSED IR LASER CRYSTALLIZATION OF AMORPHOUS SILICON FILMS

Kamil Çınar[a] and Alpan Bek[a]
[a] *Middle East Technical University, Department of Physics, Dumlupinar Blv. 1, Ankara 06800, Turkey*
e-mail: bek@metu.edu.tr

In this work, a 1064 nm nanosecond pulsed laser was used to crystallize amorphous silicon (a-Si) films with thicknesses in order of 1 micrometer. Laser crystallization (LC) of a-Si layers is an active interest in applied thin film research [1-4]. Great majority of studies on thin-film LC process are mainly focused on utilization of continuous wave lasers. In addition, LC process is typically conducted at elevated temperatures of substrates in order to avoid defects and attain improved crystallinity in device applications such as fabrication of solar cells. The LC process with infrared irradiation is typically sustained with optical power in kW ranges [1,2]. In solar cell related applications, thicknesses of deposited a-Si films reside in the range of tens of micrometers for achieving significant absorption and photoconversion. In our study, the thicknesses of deposited a-Si layers were decreased down to 1 micrometer range and the LC was performed on room temperature substrates. We were able to control crystallization process by a number of independent laser parameters, since the pulsed lasers provide freedom in adjustment of the pulse-overlap, average irradiation power and scan speed [5] (Fig. 1).

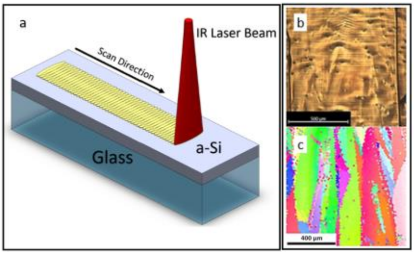


Figure 1: **a)** scheme of the laser crystallization, **b)** optical image of the crystallized film, **c)** Electron back-scatter diffraction map of the same film.

The influence of pulse overlap, presence and choice of intermediate dielectric layer between glass substrate and a-Si film were investigated in detail [6-7]. Moreover, various heterojunction solar cell device structures were designed and fabricated on p-type LC Si films by subsequent deposition of n-type a-Si. These devices are found to exhibit promising photoresponse.

[1] A. Slaoui et al., *Proc. of SPIE*, **2012**, 8473, pages.
[2] M. Weizman et al., *Sol. Energy Mater. Sol. Cells*, **2014**, 120, 521–525.
[3] J. Haschke et al., *IEEE J. Photovoltaics*, **2015**, 5, 1001–1005.
[4] J. Dore et al., *IEEE J. Photovoltaics*, **2015**, 5, 9–16.
[5] V. Türker et al., *Instruments*, **2019**, 3(2), 31.
[6] K. Çınar et al., *ACS Omega*, **2018**, 3, 5846−5852.
[7] K. Çınar et al., *J. Phys. Chem. C*, **2020**, 124, 976−985.

SYNERGISTIC EFFECTS DURING THE OBTAINING OF POLYVINYLPYRROLIDONE NICKEL-FILLED COPOLYMERS

B. Berezhnyy[1*], O. Grytsenko[1], O. Suberlyak[1], N. Baran[1], A. Fechan[1]
[1]*Lviv Polytechnic National University, 12 Bandera str., Lviv 79013, Ukraine*
e-mail: bersebog@gmail.com

The purpose of this work was to investigate the synergistic influence of the polymer matrix and the Ni(0) particles’ metal surface on the regularities of formation, structure and properties of Polyvinylpyrrolidone (PVP) nickel-filled copolymers.

Nickel-filled copolymers of 2-hydroxyethylmethacrylate (HEMA) with PVP (Ni/pHEMA-gr-PVP) and their hydrogels were used as a research object. Ni/pHEMA-gr-PVP copolymers were obtained by polymerization filling of fine Ni(0) particles, which were previously received, and the developed method of polymerization with simultaneous Ni^{2+} chemical reduction.

The influence of the metallic surface on the forming process of the composite is manifested during the synthesis of the polymer matrix. It is established that in the presence of Ni(0) particles, the polymerization of HEMA/PVP compositions occurs with a high rate at room temperature, in air, without additional initiators. The opposite effect is observed during the combination of polymerization and Ni^{2+} reduction processes – the rate of polymerization decreases. At the same time, the rate of nickel ion recovery process is increasing.

Grafted crosslinked copolymer is obtained during the copolymerization of HEMA with PVP, that was confirmed by ATR FTIR and thermogravimetric analyzes. By means of dynamic mechanical thermal analysis, it is shown, that with the presence of Ni(0), a different structure of the polymer network is formed in the interphase layer on the particles’ metal surface and in the polymer’ volume. The interaction at the interface polymer-metal and the Ni(0) surface participation in the formation of the polymer’ chemical structure manifests as a positive influence on the efficiency and a PVP grafting degree and the decrease in the molecular weight of the polymer chain fragment between crosslinks, which is a consequence of strength characteristics improvement.

During the Ni^{2+} reduction in the polymerization process of HEMA/PVP compositions, the Ni(0) nanoparticles are obtained simultaneously with the polymer matrix formation, which enables them to achieve a better, uniform distribution and obtain a composite with isotropic properties. This effect is achieved as a result of the ternary HEMA/Ni^{2+}/PVP complex formation and the Ni^{2+} ions coordination, with following stabilization of the formed Ni(0) particles.

It is established that the properties’ nature of the change of Ni/pHEMA-gr-PVP copolymers mainly depends on the method of introducing the filler into the polymer matrix, which is especially manifested in the composites’ sorption ability and electrical conductivity.

PROPERTIES OF MICROWAVE CURED EPOXY-ANHYDRIDE COMPOUNDS

O. Bilogubka
Scientific Research Center of Criminalistics, Ministry of Internal Affairs of Ukraine
National Guard str.14, Ivano-Frankivsk, 76000, Ukraine
e-mail: balan_o@i.ua

Epoxy compounds are usefulin many applications. Epoxy polymer curing is a long process andusually requires high temperatures. The microwavefield is knownto accelerate many chemical reactions. This method isespecially effective in polymers since heating occurs uniformly throughout the volume of the polymermatter. In this paper, properties of epoxy-anhydride compounds cured ina microwave field are investigated. The studied object was ED-20 oligomer cured with phthalic and maleic anhydrides. Curing was performed in a microwave oven with frequency of 2.45 GHz and power of 600 and 1000 Watts. Properties of the obtained polymers were compared with those of thermally cured for 24 hours at 120° C (for phthalic anhydride) and for 5 hours at temperature of 150° C (for maleic anhydride). The quality of the polymers was evaluated using thermal mechanical and physics-mechanical properties. Thermomechanical properties of the obtained compounds were measuredunder uniaxial compression P = 106 N/m^2 and at heating rate of 1.5 degree/minute. The samples were cylinders 9 mm of high and 8 mm in diameter. Dependences of relative deformation on temperature were registered.The obtained thermal mechanical curves provide glass transition temperature (T_g), molecular mass of the segment between the crosslinks(M_s) and modulus of high elasticity (E). Microwave curing at power of 600 and 1000 W results in suitable values of glass transition temperature andmodulus of high elasticity. The decrease in molecular mass between the crosslinks indicates an increase in the crosslink density of the polymer. Microhardness and compressive strengthof the obtained polymers were evaluated as well. It is shown that the microhardness value is 19-24 kg/mm^{2}and 12-23 kg/mm^{2}for the polymers cured with phthalic anhydride and maleic anhydride, respectively. The fracture load during compression is 13.5-14.5 kg/cm^2 and 11.3-12.3 kg/cm^{2}for polymers curedwith phthalic anhydride and maleic anhydride, respectively. The conclusion is that epoxy-anhydride compounds are rapidly cured in the microwave field. Thermal mechanical and physics mechanical parameters are comparable with those of thermally cured compounds.

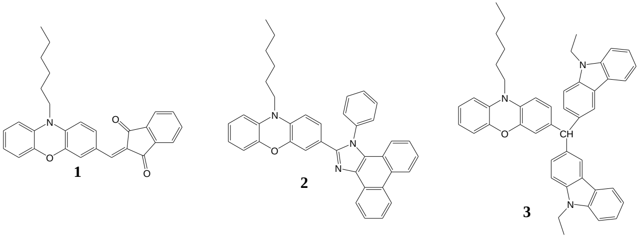
NEW STRUCTURE HOST MATERIALS FOR PHOSPHORESCENT OLED DEVICES

Dovydas Blazevicius[a], Daiva Tavgeniene[a], Marius Eidimtas[a], Gintare Krucaite[a], Baohua Zhang[b], Simona Sutkuviene[c,d] and Saulius Grigalevicius[a]

[a]Department of Polymer Chemistry and Technology, Kaunas University of Technology,
Radvilenu plentas 19, LT50254, Kaunas, Lithuania
[b]Center for Advanced Analytical Science, c/o School of Chemistry and Chemical Engineering,
Guangzhou University, Guangzhou 510006, P.R. China
[c]Department of Biochemistry, Faculty of Medicine, Lithuanian University of Health Sciences,
Tilzes str. 18, LT47181, Kaunas, Lithuania
e-mail: dovydas.blazevicius@ktu.lt

In the phosphorescent devices, to reduce quenching associated with relatively long excited-state lifetimes of triplet emitters and triplet-triplet annihilation etc., triplet emitters are normally used as emitting guests in a host material, and thus suitable hosts are widely investigated for the phosphorescent devices [1-2].

The structure of phenoxazine-based host materials **1-3** shown in Scheme 1.



Scheme 1.

New electro-active materials were synthesised using phenoxazine as electron donor fragment connected with various electron acceptors or donors. Some of the materials formed homogeneous solid amorphous films with glass transition temperatures of 75 -93 ^{o}C. Layers of the synthesized compounds showed ionization potentials of 5.24-5.56 eV. The compounds, which formed homogenous amorphous layers, were tested as host materials for green phosphorescent OLEDs. The device with the host of 3-[bis(9-ethylcarbazol-3-yl)methyl)-10-hexylphenoxazine exhibited the best overall performance. The efficient green OLED using the host demonstrated low turn-on voltage of 3.1 V, a maximum brightness of 5366 cd/m^2, external quantum efficiency exceeding 5.9 % and maximum current efficiency of 18.3 cd/A. For the technically important brightness of 1000 cd/m^2 an efficiency above 15.7 cd/A (4.9 %) was detected in the device.

Reference:

[1] K. S. Yook, J. Y. Lee, *Advandecd Materials*., **2014**, 26, 4218.

[2] E. Holder, B.M.W. Langeveld, U. S. Schubert, *Advandecd Materials*., **2005**, 17, 1109.

Acknowledgements. The OLED materials were developed in the frame of project funded by a grant No. S-MIP-17-64 from the Research Council of Lithuania.

DESIGN OF PLASTIC SCINTILLATORS FOR DETECTION OF VARIOUS TYPES OF RADIATION

V.N. Bliznyuk[a], A.F.Seliman[a], N.A.Derevyanko[b], A.A.Ishchenko[b], S.M.Husson[a], T.A.DeVol[a]
[a] *Clemson University, Clemson, South Carolina 29634 USA*
[b] *Institute of Organic Chemistry NASU, 5 Murmanskaya Str., Kiev 02660, Ukraine*

e-mail: vbliznу@clemson.edu

Plastic scintillators (PS) play important role in modern radiation detectors and sensors. Our group has developed recently new organic fluorophores with functional vinyl groups enabling their copolymerization with the matrix monomer (styrene, vinyl toluene, vinyl carbazole etc.) [1,2]. This approach allows not only improving the efficiency of bulk scintillators via reduction of fluorophore aggregation and better coupling of the fluorophore molecules to the matrix but also opens new applications in microfluidics, sensors and other micro/nano-scale devices. Monolayer coatings or brush films can be deposited on photolithography patterns or various nanoparticles by surface-initiated atom transfer radical polymerization [3]. We demonstrate in our presentation how scaling down of the traditional plastic scintillators to microfluidic sensors and core-shell nanoparticles can be used for monitoring radioactive pollutions in nuclear forensics and homeland security applications. We will show also that our approach enables preparation of bulk scintillators targeting gamma ray detection via addition of high-Z nanoparticles or organometallic compounds (Fig. 1). Possible modifications of the system to enhance n/γ (or α/β) pulse shape discrimination (PSD) function will be discussed.

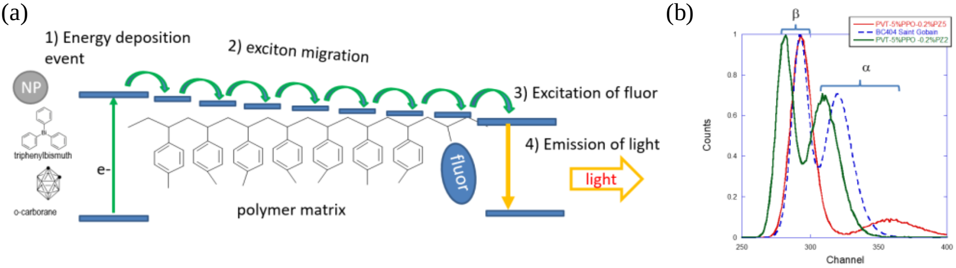


Fig. 1. (a) Scheme of conversion of the radiation energy into the energy of visible light during operation of PS. Higher sensitivity to gamma-ray and neutron radiation is achieved via inclusion of high-Z nanoparticles or organo-metallic compounds, or boron compounds, respectively; (b) an example of α/β PSD spectra recorded using PSs based on pyrazoline fluorophores in comparison to a commercial BC404 bulk scintillator.

[1] V.N.Bliznyuk A.F.Seliman, A.A.Ishchenko, N.A.Derevyanko, T.A.DeVol, *ACS Appl. Mater. & Interfaces*, 2016, 8 **(**20) 12843-12851.
[2] A.F.Seliman, V.N.Bliznyuk, S.M.Husson, T.A.DeVol, *J.Mater.Chem. C*, 2015, 3 (27) 7053-7061.
[3] V.N.Bliznyuk, A.F.Seliman, S.M.Husson, Y.M.Lvov, T.A.DeVol, *Macromol. Mater. Eng.*, 2018, 303 (6) 1700651.

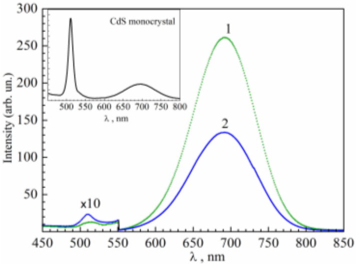
LUMINESCENT INVESTIGATIONS OF CADMIUM SULFIDE NANOWHISKERS

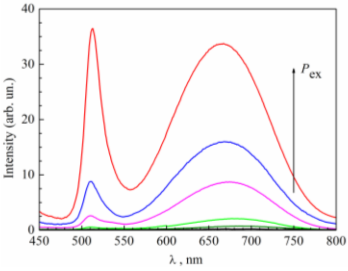
A. Bogoslovska, D. Grynko, E. Bortchagovsky
Institute of Semiconductor Physics of NAS of Ukraine, pr.Nauki 41, Kyiv 03028, Ukraine
e-mail: alla.bogoslovska@gmail.com

Nanostructured materials attract great scientific and technical interest, due to their unique properties and possibilities of utilization in novel promising optoelectronic devices, solar cell, display panel and so on. Optical properties of nanostructures may be very different from the bulk ones. Even beside of quantum-size effects, high ratio of surface to the volume of such structures has big influence on luminescent and optical properties.

We grow CdS nanowhiskers from gas phase in home-built equipment and investigated their luminescent properties depending on technological growth parameters and excitation conditions. High crystallinity of our structures was confirmed by XRD data. Luminescence spectra measured with the excitation by semiconductor laser of 407 nm exhibit two band visible for the bulk material too. The narrow band centered at 510 nm attribute to near band edge (NBE) emission of CdS nanowhiskers (the bandgap of CdS is 2.42 eV at room temperature). There are many and even controversial explanations of the origin of broad emission ranging from 580 nm to 780 nm. One of them prescribes this band to the surface states what is confirmed by our results.

PL spectra of two samples with different diameter of CdS whiskers are shown in Fig.1 together with the spectrum of bulk CdS included in the insert. The ratio of the intensity PL of the defect band to the intensity of the edge band luminescence is noticeably bigger for whiskers with smaller diameter (1), which has bigger ratio of the surface region to the bulk. Luminescence of the bulk crystal confirms this behavior demonstrating only weak long-wavelength luminescence. Fig.2 exhibits the evolution of PL spectra CdS nanowhiskers with increased excitation power. If the intensity of the long-wavelength emission grows linearly with raising the excitation power, the intensity of the NBE emission grows superlinearly exceeding the intensity of the defect band after some moment. As the result the emitting color of CdS nanowhiskers changes from red to green.





The color-tunable photoluminescence of CdS nanowhiskers may have potential applications in color tunable nanodevices.

CRYSTALLINE SILICON WAFER SLICING BY DEEP SUBSURFACE LASER INDUCED MODIFICATION FOLLOWED BY SELECTIVE CHEMICAL ETCHING

Mona Zolfaghari Borra[a,b], Hisham Nasser[a], Behrad Radfar[a,b], Ihor Pavlov[a,c,d], Rasit Turan[a,b,d], Alpan Bek[a,b,d]
[a] *The Center for Solar Energy Research and Applications (GÜNAM), Middle East Technical University, 06800, Ankara, Turkey*
[b] *Micro and Nanotechnology Graduate Program, Middle East Technical University, 06800, Ankara, Turkey*
[c] *Institute of Physics of the NAS of Ukraine, Kyiv, Ukraine*
[d] *Department of Physics, Middle East Technical University, 06800, Ankara, Turkey*
e-mail: mborra@metu.edu.tr

In this contribution, we demonstrate the use of laser-induced silicon slicing (LASIS) technique followed by wet chemical selective etching. This technique allows the fabrication of crystalline silicon (c-Si) slices or wafers with minimum loss of the material [1]. In LASIS method, a nanosecond-pulsed fiber laser operating at 1.55 μm wavelength is focused deep in Si subsurface and induces structural modifications near the focal point due to multiphoton absorption. The raster scan of the focal position inside c-Si sample, positioned in cross-sectional plane with respect to laser beam, produces a quasi-2D modified Si region. The modified Si region is then etched by cupper nitrite (Cu $(NO_3)_2$)-based selective chemical etchant which selectively targets the laser-modified regions. In order to achieve high etch rates along with smooth and defect-free surfaces; different etchant components concentrations and etch durations were investigated.

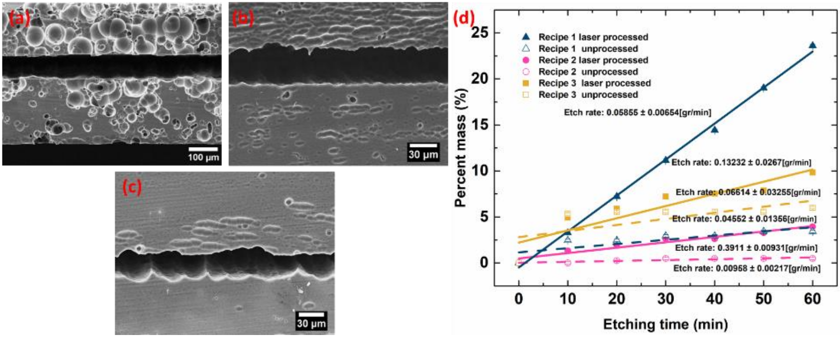


Fig. 1 (a) Cross-sectional SEM images of laser-processed and chemically treated c-Si with different selective etchant recipes : 1 (a), 2 (b), 3 (c). Etched Si percent mass as a function of etch duration is given in (d).

Figures 1 (a-c) display effect of different etch recipes on the morphology of laser-modified regions together with non-modified Si regions. Figure 1(d) shows the etched percent mass, which is defined as the ratio of the etched mass over the total mass, as a function of etch duration. It can be seen that the etch rate difference between laser processed and unprocessed regions for recipe 1 is higher than that of recipes 2 and 3. On the one hand, using a high HF concentration in recipe 1 resulted in more defective surfaces (see Figure 1 (a) /Recipe 1), and reducing the amount of HF resulted in less defect regions (see Figure 1 (b) /Recipe 2). On the other hand, increasing the concentrations of CH_3COOH and $Cu(NO_3)_2$ with moderate amount of HF resulted in least fraction of defect regions associated with increasing etch rate (see Figure 1 (c) and (d)/Recipe 3). Figure 2 shows cross-sectional SEM images of laser-processed c-Si wafers at different stages.

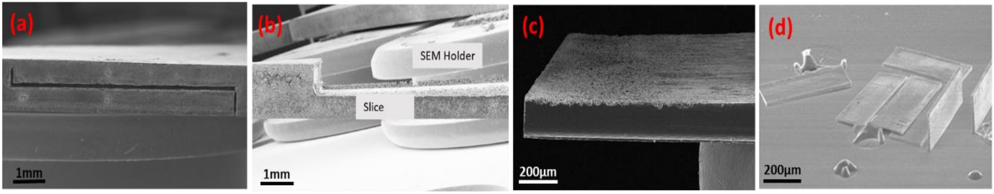


Fig. 2 Cross-sectional SEM images of laser-processed c-Si wafer at different stages : after 20 minutes etching (a), slice formation after 3 hours etching (b), (c), and (d).

Obtained c-Si slices can be utilized in wide range of applications including photovoltaic solar cells, Si based optoelectronic devices, and photonic crystals.

[1] O. Tokel, A. Turnalı, G. Makey, P. Elahi, T. Çolakoğlu, E. Ergeçen, Ö. Yavuz, R. Hübner, M. Z. Borra, I. Pavlov, A. Bek, R. Turan, D. K. Kesim, S. Tozburun, S. Ilday, F. O. Ilday “In-chip microstructures and photonic devices fabricated by nonlinear laser lithography deep inside silicon” Nature Photonics **11**, 639 (2017)

PHENOL-BASED OLIGOMERS WITH REACTIVE FUNCTIONAL GROUPS

Michael Bratychak
Lviv Polytechnic National University, 12 Bandery St., Lviv 79013, Ukraine
e-mail: mbratychak@gmail.com

The phenol-based oligomers (PhBO) are widely used to produce products with high thermal stability, heat insulation and aggressive media resistance. In order to improve the operational characteristics of PhBO, as well as to combine them with other polymer materials, phenol-based oligomers are modified with various low- and high-molecular compounds.

In this work we created new PhBO with unsaturated double bonds or labile peroxy groups in the side chains.

The initial compounds for the synthesis were novolac phenol-formaldehyde resin (NPhFR) and polyglycidyl phenol-formaldehyde resin (PGPhFR).

Glycidyl methacrylate (GMA), methacrylic acid (MA) and peroxy derivative of ED-24 epoxy resin were used as the low-molecular compounds.

Synthesis of phenol-formaldehyde oligomers with methacrylic fragments

The new compounds were synthesized by two ways:

1) NPhFR was used as an initial compound. GMA, which contains methacrylic fragment in its structure, was a modifier (1.5 mol/phenolic group). A catalyst was KOH in amount of 0.6 mol per one phenolic group of the initial resin. The reaction temperature was 333 K, reaction time – 6 h. The reaction was carried out in the medium of inert gas using isopropyl alcohol as the reaction medium. The resulting product has the molecular weight of 640 g/mol and bromine number 22.9 g Br2/100 g product.

2) PGPhFR was the initial resin and MA (1.0 mol/g-eq epoxy group) was a modifier. Benzyl triethylammonium chloride (BTEAC) in amount of 0.2 mol/g-eq epoxy group, 60% aqueous solution, was used as a catalyst. The reaction temperature was 353 K, reaction time – 6 h. To prevent polymerization by double bonds, inert gas was used and toluene was a reaction medium. The resulting product has the molecular weight of 590 g/mol and bromine number 28.1 g Br2/100 g product.

Synthesis of phenol-formaldehyde oligomers with peroxy groups

To obtain phenol-based oligomers with peroxy groups novolac phenolformaldehyde resin was used. Peroxy derivative of ED-24 epoxy resin was used as a modifier in amount of 0.5 mol/phenolic group. The catalyst was KOH in amount of 0.4 mol/phenolic group. The reaction was carried out at 323 K for 6 h in the medium of isopropyl alcohol. The synthesized oligomer has the molecular weight of 750 g/mol and active oxygen content of 1.6 %.

DEFINING THE CONDITIONS FOR THE FORMATION OF OXIDE FILMS DURING THE ELECTROCHEMICAL OXYDATION OF THE Ti6Al4V ALLOY IN ETHYLENEGLYCOL SOLUTIONS

O. Bukhinik[a], S. Gura[b], A. Pilipenko[a]
[a]*National Technical University «Kharkiv Polytechnic Institute», Kyrpychova str., 2,*
Kharkiv, Ukraine, 61002
[b]*National University of Civil Protection of Ukraine, Chernyshevska str., 94,*
Kharkiv, Ukraine, 61023
e-mail: opilipenko1984@gmail.com

The titanium grade Ti6Al4V alloy is used for the production of critical items and it combines both an increased specific strength and an increased corrosion resistance. The alloy corrosion resistance is ensured by the formation of the natural ultrathin oxide film of 5 to 6 nm thick that is formed during the exposure of the alloy surface to the ambient oxygen. This film provides an abrupt decrease in the chemical activity of an alloy and it results in the metal passivation in most of oxidizing environments.

A passive film discontinuity caused by activating ions that are available in the working media or by mechanical wear may result in the catastrophically fast metal failure. The alloy surface modification is one of the methods used for an increase in the alloy corrosion resistance. This method consists in the electrochemical oxidation required to get thicker oxide films. The resultant film thickness can vary in the range of 0.1 to 200 µm that contributes to a deeper alloy passivation and a decreased corrosive failure rate.

The thickness and structure of oxide film that is formed using the method of electrochemical oxidation are mainly defined by the electrolyte nature. A failure of electrolyte components to interact with the film results in the formation of semi-porous films of a barrier type. An addition of activating ions to the electrolyte facilitates the formation of the double-layer films that include porous and barrier parts.

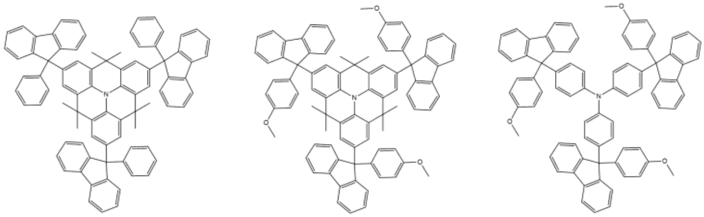
The most promising approach to the solution of this problem is to make use of organic electrolytes with surface-active properties that enable the oxidation with the final outcome in the form of porous oxide films with the uniform pore distribution and it should be noted that these formed pores have a specific diameter. The films of this type can be used not only for an increase in the item chemical resistance but also for the development of surface by the oxide layer that displays biocompatibility and bioinertness properties.

The data obtained during the investigation of the oxidation of the Ti6Al4V alloy in ethylene glycol electrolytes allowed us to establish the formation modes for semiporous and double-layer oxide films, study both the kinetics of electrode reactions and the passive layer formation dynamics. Electrochemical investigation data were supported by composition analysis data and the alloy surface photomicrography that enabled the determination of the effect of electrolysis conditions on the oxide film structure.

SYNTHESIS AND PROPERTYS OF ARYLFLUORENYL SUBSTITUTED DERIVATIVES OF BRIDGED-TRIPHENYLAMINE AND TRIPHENYLAMINE FOR OPTOELECTRONIC APPLICATIONS

M. Cekaviciute[a], J. Simokaitiene[a], J.V. Grazulevicius[a], D. Volyniuk[a], G. Sini[b]
[a]*Department of Polymer Chemistry and Technology, Kaunas University of Technology, Radvilenu pl. 19, 50254 Kaunas, Lithuania*
[b]*Laboratoire de Physicochimie des Polymeres et des Interfaces, EA 2528 Universite de Cergy-Pontoise, 5 mail Gay-Lussac, Cergy-Pontoise Cedex, France*
e-mail: monika.cekaviciute@ktu.lt

Derivatives of triphenylamine represent one of the largest and one of the most widely studied classes of organic electroactive materials [1,2]. They are widely used in electro photographic photoreceptors, organic light emitting diodes, solar cells. Bridged-triphenylamines were studied as planar hole transporting materials for electroluminescent devices and perovskite solar cells [3]. In this presentation, we report on synthesis and investigation of properties of new glass-forming arylfuorenyl substituted derivatives of triphenylamine and methylene-bridged triphenylamine.



The target compounds were synthesized by single-step procedure, i.e. by acid promoted Friedel-Crafts-type substitution reaction [4]. They were identified by mass-, IR- and ^{1}H, ^{13}C NMR spectrometries. The synthesized derivatives exhibited high thermal stability with the onsets of thermal degradation above 443°C and formed glasses with glass transition temperatures being in the range of 171–187 °C. The ionization potentials of the synthesized compounds were close and ranged from 5.30 eV to 5.36 eV as established by cyclic voltammetry. Time-of-flight hole mobilities in the solid layers of the synthesized triphenylamine derivatives exceeded 10^{-3} $cm^2/V{\cdot}s$ at an electric field of 6.4×10^5 V/cm.

This work was supported by the Research Council of Lithuania (Grant No S-LU-20-12).

[1] A. Iwan, D. Sek, *Prog.Polym.Sci.*, **2011**, 36, 1277–1325.
[2] Y. Shirota, H. Kageyama, *Chem. Rev.*, **2007**, 107, 953–1010.
[3] H. Choi, S. Park, S. Paek, P. Ekanayake, et al., *J.Mater.Chem.A*, **2014**, 2, 19136–19140.
[4] P.-I. Shih, C.-H. Chien, F.-I. Wu, C.-F. Shu, *Adv.Funct.Mater.*, **2007**, 17, 3514–3520.

THERMODYNAMIC OF METHYLENE BLUE ADSORPTION ON THE HYBRID TiO2 / DIATOMITE NANOCOMPOSITE

Datsko T., Zelentsov V.
The Institute of Applied Physics of Moldova, Chisinau, Republic of Moldova
e-mail: datsko.tatiana@yandex.ru

Heterogeneous photocatalysis is a complex physico-chemical process that occurs in an aqueous system and includes the adsorption of molecules on the surface of a solid, the absorption of UV energy and the oxidation-reduction reaction.

The main oxidation - reduction reaction takes place on the catalyst surface and substantially depends on its adsorption-structural properties and is often determined by them.

Therefore, the adsorption properties of the catalyst play an important role in the photocatalytic decomposition of organic pollutants.

The hybrid photocatalyst DTD based on nanosized TiO_2 (anatase form) grafted on diatomite surface was prepared via heterogeneous hydrolysis of $TiCl_4$ as a precursor of TiO_2 in the diatomite suspension at room temperature and normal pressure. The obtained product was further washed, dried and calcined at 450^{o}C for anatase phase development. The amount of titania in the product is about 20%.

In the paper the thermodynamic parameters of methylene blue (MB) dye adsorption (the change in Gibbs standard free energy, ΔG^{o}, enthalpy, ΔH^{o} and entropy, ΔS^{o}) on the DTD have been calculated using the following equations:

$$\Delta G^{o} = -RT \ln K_d$$

where K_d is the distribution coefficient, R is the universal gas constant (8.314 J mol-1 K-1) and T is the absolute temperature in K.

$$K_d = \frac{C_s}{C_e}$$

where C_s and C_e is the concentration of the adsorbate on the sorbent surface and in bulk solution at equilibrium, mg·L^{-1}.

The negative values of the Gibbs free standard energy ΔG^{o} (-0.714, -1.159, -2.296 kJ·mol^{-1} at 293, 303, and 313K, respectively) shows that the adsorption of MB on the DTD is spontaneous. Positive value of ΔH^{o} (22.57 kJ·mol$_{-1}$) characteristic of the endothermic process, were relatively high, which indicates that the interaction between the sorbent active sites and the adsorbate molecules was not only physical, but also chemical.

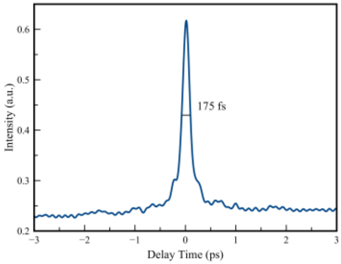
A negative ΔS^{o} value (-79 J·mol^{-1}·K^{-1}) indicates a decrease in the disorder of the system at the solid / solution interface during the adsorption of MB on the photocatalyst.

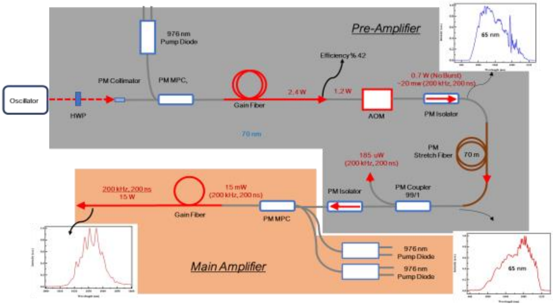
BURST MODE ULTRAFAST LASER WITH NOVEL PULSE STRECHING FOR MICROMACHINING

Mahmut Emre Yağcı[1], Volkan Türker[1], Svitlana Pavlova[1], Erşan Tunçkol[1], Semih Koray Eken[1], Ihor Pavlov[2]
[1] *FiberLAST Inc., METU Teknokent, Ankara 06800, Turkey*
[2] *Department of Physics, Middle East Technical University, Ankara 06800, Turkey*
e-mail: emre.yagci@fiberlast.com.tr , volkan.turker@fiberlast.com.tr

The ultrafast laser serves as an advanced tool for material processing with greatly reduced or absent heat effects in fabrication of miniaturized devices, precision micromachining, self-assembly techniques, highly controlled surface texturing and pulsed laser deposition of high-quality films. The main obstacle to use of ultrafast laser micromachining is improvement of the ablation speed. While scaling up the average power has allowed increases in repetition rate at pulse energies high enough for micromachining, the returns of this approach is severely limited in practice by the speeds of the devices, such as galvanometer-based scanners that can be used for beam positioning [1-3]. A very interesting and until recently under-appreciated technique is to generate bursts of high repetition rate pulses at a lower overall repetition rate [4-5].

The main goal of this research is the development of a unique burst-mode femtosecond Yb-doped fiber laser system operating around 1 μm central wavelength and its application to micromachining and processing of various industrially relevant materials. In order to achieve femtosecond pulse bursts, which is compressible to 100-200 fs with output energies of up to 7 μJ per pulse and at least 70 μJ per burst, a novel pulse shaping mechanism that is distinct from the well-known chirped pulse amplification (CPA) and nonlinear chirped pulse amplification schemes was developed.





This was enabled by development of specialty component which is GRISM for third order dispersion (TOD) and additional nonlinearity reduction schemes was applied and realized without any setbacks in terms of fiber integration of the system. All-important burst parameters of the laser, e.g., number of bursts, intra-burst repetition rate and the repetition of the bursts are fully adjustable with FPGA based electronic control card and PC command interface, thus offering precisely controllable material processing conditions. This laser system was developed into an industrial prototype, which was tested long term. Briefly, it was achieved to reach 7 μJ per pulse and 300 μJ per burst energy at 1030 nm central wavelength. The maximum average power of this laser is 15 W and intra-burst repetition rate is around 95 MHz.

DEVELOPMENT OF ANTIMICROBIAL MATERIALS BASED ON PLA/MEDITERRANEAN PROPOLIS AND THYMUS VULGARIS ESSENTIAL OIL

Hocine Djidjelli, Nacera Chibani, Nadjet Ardjoum
Université de Bejaia, Laboratoire des Matériaux Polymères Avancés 06000, Algérie
e-mail: hocdjidj@yahoo.fr

Antimicrobial films based on polylactic acid (PLA) were developed by incorporated *thymus vulgaris* essential oil Thymol (EOs) (2%) v/v with different concentration of ethanolic extract of Mediterranean propolis (EEP) (5-10%) w/w. The results of antibacterial and antifungal test indicated that (EEP) was showed a high antibacterial and antifungal effect with (12.1 mm and 11.58 mm) against *Staphylococcus aureus* and *Penicilliumsp*, respectively. FTIR analysis exhibited a successful dispersion of(EEP) andThymol(EOs) in polymer matrix. The mechanical test revealed a decreasing of tensile strength and elastic modulus from the active films. But the percentage of elongation increased. In addition, the incorporation of (EEP) concentration was resulted a darker color films. Antimicrobial activity of films exhibited thatfilms containing (10%) w/w of (EEP) was inhibited the growth of *C.albicans* and the combination of (EEP) and (EOs) in PLA matrix showed asynergistic effect against*E.coli*.

OPTIMISATION OF LASER-INDUCED SURFACE STRUCTURES FOR SENSITIVITY OF THEIR SPECTRAL CHARACTERISTICS TO CHANGES IN THE ENVIRONMENT

I. Dmitruk[a], N. Berezovska[a], O. Yeshchenko[a], O. Stanovyi[a], E. Hrabovsky[a], P. Teselko[a],
A. Dmytruk[b], I. Blonskyi[b]
[a]*Taras Shevchenko National University of Kyiv. Volodymyrska Street, 64/13, Kyiv-01601, Ukraine*
[b]*Photon Processes Department, Institute of Physics of the NAS of Ukraine. Prospect Nauki, 46, Kyiv-03039, Ukraine*
e-mail: igor_dmitruk@univ.kiev.ua

The report deals with the demonstration of practical applications of laser-induced periodic surface structures (LIPSS) for amplifying the electric field of the light wave in the near-surface region of the sample and, as a consequence, an enhancing of such phenomena as absorption, photoluminescence (PL), Raman scattering.

Ti:sapphire femtosecond laser with a central wavelength of 800 nm and a pulse duration of 120-130 fs (full duration at half-height) has been used for the fabrication of LIPPS on nobel metals (Ag), semiconductors (ZnSe). Scanning electron microscopy (SEM) has been used to study the morphology of the treated surfaces.

In this research, it has been analyzed the LIPSS on noble metals characterized by the presence of metal nanoparticles (NPs), which were formed as a result of the ablation process under the laser structuring, or were deposited on the surface. This combination of carriers of surface plasmon polaritons (SPP) and local plasmon resonators provided the complementarity of the effects of amplification of the field of an electromagnetic wave.

Surface-enhanced Raman scattering (SERS) on Ag LIPPS has been demonstrated for the vibrational modes of the Rhodamine 6G and Methylene blue dyes. The observed SERS of dyes is mainly due to the strong electric fields near the Ag LIPPS caused by localized plasmon resonance in the metal submicron- and nano-structures (metal NPs on the surface due to the laser ablation). This is so-called electromagnetic amplification.

The use of non-spherical Ag NPs deposited on the Ag LIPPS provided the plasmon enhancement of the PL of such nucleotide as 5’-deoxyadenosine-monophosphate (dAMP) with a PL gain factor up to 1120 times. The generation of hot spots near the sharp edges of LIPSS and non-spherical Ag NPs has a crucial role for this amplification. Thus, the created structures are promising for the highly sensitive detection of the changes in the near surface area of the sample, in particular the appearance of biomolecules on the sample surface.

Laser treatment of the ZnSe semiconductor surface resulted in a significant enhancement of the PL band with a maximum at 630 nm (1.92 eV) caused by a complex center containing zinc vacancy.

SOME PHYSICO-CHEMICAL ASPECTS OF THE PREPARATORY STAGES OF THE FORMATION OF SELF-CLEANING PHOTOCATALYTICALLY ACTIVE COATINGS

O. Dryuchko, D. Storozhenko, N. Bunyakina, I. Ivanytska, I. Gornitsky,
K. Kytaihora, V. Khaniukov
Poltava National Technical Yuri Kondratyuk University, Pervomaysky prospect, 24, Poltava, 36011, Ukraine, e-mail: dog.chemistry@gmail.com

A complex systematic study of the interaction of structural components in cerium subgroup lanthanide nitrate systems and representatives of the IA group (Li, Na, K) of the elements of the periodic system - precursors of modern multicomponent oxide multifunctional materials based on them - established the formation of a representative class of alkaline coordination nitrates Ln. Their composition, formation conditions, atomic crystalline structure, forms of Ln coordination polyhedral, types of ligand coordination, a number of their properties were studied using a complex of physicochemical methods: chemical, X-ray phase, X-ray structural, IR spectroscopic, crystal-optical, thermo graphic, SHG laser radiation. The data obtained are the basis for identifying, identifying, monitoring the phase state of processing facilities in the preparatory stages when forming self-cleaning coating layers of building construction materials using innovative technologies using nanostructured composite systems of lanthanides and transition elements with photo catalytically active and hydrophilic properties, various combined methods of their activation and establishing technological and functional dependencies yaemogo modify the properties of the products obtained.

Photocatalytically active coatings are precipitated using a variety of technologies, such as sol-gel, spray pyrolysis, chemical or steam vapor deposition, and magnetron sputtering. Regulations are now being implemented using “solution burning” methods.

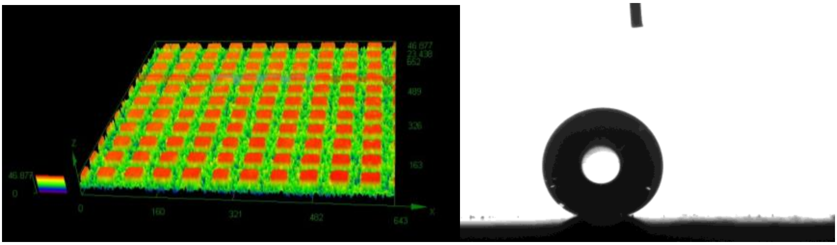
A promising class of photocatalytically active rare earth oxides and titanium oxide materials that can act as alternatives to existing developments are nanostructured layered perovskite-like compounds and solid solutions based on them. Depending on their composition and structure, they have a wide range of physicochemical properties. The perovskite-like layered titanates presented in this work belong to the homologous series $(Me, Ln)_{n+1}Ti_nO_{3n+1}$ – the Raddlesden-Popper phases, where Me is H, Li, Na, K, Rb, Cs; Ln – La, Nd; n is the number of perovskite nanolayers with a thickness of about 0.5 nm.

The obtained system of knowledge about transformation processes in systems of REE-containing nitrate precursors and crystal-chemical properties of samples of coordination nitrates Ln is of particular value in the formation of nanostructured layered perovskite-like compounds of lanthanides and transition elements (including their titanium); when establishing technological and functional dependencies between the method of preparation, the variability of the method of activation of technological systems, the methodology of production of the target product and its phase composition, lattice parameters, the specific surface area, the morphology of the constituent particles, the activity of layers of self-purifying compositions with hydrophilic structures and special structural elements; in practical implementation of innovative projects of decomposition of water for the purposes of hydrogen production, decomposition of toxic organic substances in solutions and air, incomplete oxidation of carbohydrates; upon receipt of other perovskite-like phases by ion exchange reactions and in other fields.

PICOSECOND LASER PROCESSING OF STAINLESS STEEL FOR SUPERHYDROPHOBIC SURFACE FABRICATING.

Dupliak Ivan[a], Yuchen Liang[a], Guozhu Yan[a], Fenping Li[a], Ivaniuk Khystyna[b]
[a] *Wenzhou University Institute of Laser and Optoelectronic Intelligent Manufacturing*
Ocean Science and Technology Innovation Park, No. 19 Binhai 3rd Road, Yongxing Street, Longwan District, Wenzhou, Zhejiang, China
[b] *Lviv Polytechnic National University, Lviv, Ukraine*
e-mail: ivandupliak@gmail.com; tel.: +86 15868500795

Micro- and nano-structured metallic surfaces with special wettabilities due to important applications such as anticorrosion, oil–water separation, friction reduction, and liquid transportation are strongly studied over the past few decades[1–3]. In this work obtaining a hydrophobic metal surface is achieved by increasing the surface roughness of the material and further decrease of the contact angle of water droplets on the surface.



304 stainless steel samples with dimensions of 50 mm × 50 mm × 1 mm were used. The surface was textured by a picosecond laser system (MicroMach2040, Xi'an Micromach Technology Co.,Ltd) with 10 ps laser pulses, 10 kHz repetition rate, 515 nm wavelength.

The superhydrophobic cross-groove patterns were constructed by line-by-line laser ablation with processing parameters. The maximum contact angle of 164 ± 2.5° was reached with following parameters: laser power 2.5 W, scanning speed 10 mm/s, scanning times 1 times.

Superhydrophobic surface was fabricated 304 stainless steel on stainless steel plates using cheap fast and easy method of picosecond laser micromaching. Resived microstructure gives a stainless steel plates high anticorrosion and antibacterial properties, reduces friction which may extend the scope of this material.

1. J. Long, M. Zhong, H. Zhang, P. Fan, J. Colloid Interface Sci. (2015). doi:10.1016/j.jcis.2014.11.015.
2. T. Jiang, J. Koch, C. Unger, E. Fadeeva, A. Koroleva, Q. Zhao, B.N. Chichkov, Appl. Phys. A Mater. Sci. Process. (2012). doi:10.1007/s00339-012-6985-4.
3. Q. Pan, Y. Cao, W. Xue, D. Zhu, W. Liu, Langmuir. (2019). doi:10.1021/acs.langmuir.9b01333.

Ni-Co/SiO_2 COMPOSITES: SURFACE STRUCTURE AND MORPHOLOGY

Dyachenko A.[a], Ischenko O.[a], Goncharuk O.[b], Borysenko M.[b]
[a] *Taras Shevchenko National University of Kyiv, 64/13 Volodymyrs’ka str., Kyiv, Ukraine*
[b] *O.O. Chuiko Institute of Surface Chemistry of NAS of Ukraine, 17 General Naumov str., Kyiv, Ukraine*
e-mail: dyachenko.alla@yahoo.com

A set of bimetallic 10 wt %(Ni-Co)/SiO_2 ($Ni_{80}Co_{20}$, $Ni_{50}Co_{50}$, $Ni_{20}Co_{80}$) composites were synthesized using the solvate-stimulated modification of the fumed silica with Ni and Co nitrate solution and further calcinations at 600 °C [1]. As the result, the silica surface was modified with Ni and Co oxides. The next step of the synthesis was reduction of deposited on the silica surface metals oxide precursors in the H_2+He gases mixture up to metallic state.

XRD analysis of obtained composites showed Ni/Co metallic phases (Fig.1). SEM images of $Ni_{80}Co_{20}/SiO_2$ composite demonstrated equally distributed bimetallic particles on the silica surface. The small individual particle of deposited bimetallic particles (d≈30 nm) and large agglomerate of them (d≈220 nm) are observed (Fig 2a). It can be seen that metals are encapsulated in the silica peel (Fig. 2b). The most capsules are closed and only a few can be opened. Therefore the metals can be available on the silica surface and more reactive in heterogeneous catalytic reaction.

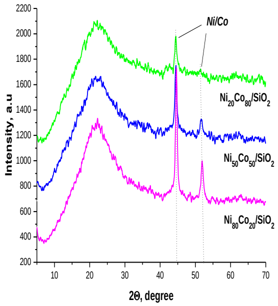
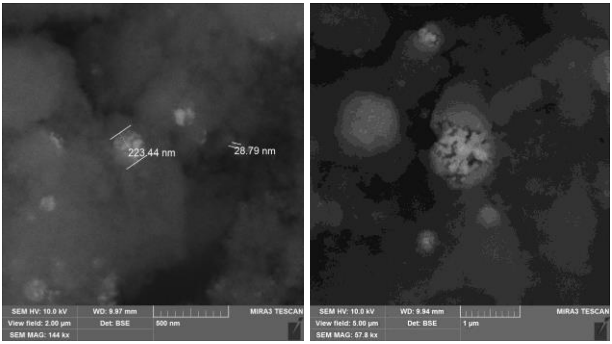


Fig.1. XRD patterns of Ni-Co/SiO_2 composites



a

b

Fig. 2. SEM images of $Ni_{80}Co_{20}/SiO_2$ composite

---

[1] O. Goncharuk et al., *J. Mol. Liq*. **2019**, 285, 397.

$PbI_2:Cd^{2+}$ NANOCLUSTERS SYNTHESIZED BY ONE-STEP DEPOSITION METHOD

O.G. Dziazko[a], I.V. Fesych[a], O.O. Bondar[a], S.A. Nedilko[a], T.A. Voitenko[a], M.A. Zelenko[a],
V.V. Lendel[a], A.P. Bukivskii[b], P.M. Bukivskii[b], O.V. Ivanov[a]
[a] *Taras Shevchenko National University of Kyiv, 64 Volodymyrska Str., Kyiv 01601, Ukraine*
[b] *Institute of Physics, NASU, 46 Prospect Nauky, Kyiv 03028, Ukraine*
e-mail: dziazko@univ.kiev.ua

Pure PbI_2 and $PbI_2:Cd^{2+}$ nanoclusters were obtained by one-step deposition method in open-air conditions. The input reagents lead iodide PbI_2 (99.9%) and cadmium iodide CdI_2 (99.9%) were dissolved in dried N,N-dimethylformamide (DMF, ≥99%) in stoichiometric proportions and ultrasonicated for 30 min at room temperature. Next, the clear bright yellow precursor solution was spin-coated on a well-cleaned silicon substrate (1×1 cm) at a speed of 3000 rotations per minute during 10 seconds and dried at 150 °C for 30 min to remove the remaining solvent.

The prepared samples were characterized by mean X-ray diffraction (XRD) in the 2θ range from 10° to 60° to determine the phase purity and crystallinity. The database of the Joint Committee on Powder Diffraction Standards (JCPDS PDF-2) was used to identify the phases.

As confirmed in the XRD studies, in the $PbI_2:Cd^{2+}$ nanoclusters two layered hexagonal 2H-polytype of PbI_2 (JCPDS card # 07-0235) as "impurities" and a mixture of four layered hexagonal 4H-polytype (JCPDS card # 33-0239) and twelve layered rhombohedral 12R-polytype (JCPDS card # 85-1600) has been observed. The pure CdI_2 crystals have four layered hexagonal structure and relate to a space group of *P63mc* symmetry. The 4H-polytype is the most stable structure of CdI_2, both at room temperature and at higher temperatures. So, in the case of $CdPbI_2$ solid solution, a polytypic transformation from 4H to 12R structure does take place [1].

In addition, the intensity of the reflexes of the PbI_2 microcrystallites at $2\theta = 12.64°$, 25.87°, 38.58° and 52.27°, where assigned to the diffraction planes (001), (002), (003) and (004) respectively, is higher in comparison with analogous reflexes of standard pattern (JCPDS card # 07-0235). These XRD results showed that in general the PbI_2 nanoclusters growth was oriented along [00l] direction. Formation of such highly oriented crystalline PbI_2 hexagons in the CdI_2 matrix may be because of the use of DMF, polar solvent containing electronegative oxygen atoms.

The obtained $Pb_{0.3}Cd_{0.7}I_2$ nanoclusters can be considered as novel promising semiconductor materials for the development of efective inexpensive scintillator detectors for biomedical and industrial applications.

[1] B. Kumar, N. Sinha, *Cryst. Res. Technol.* **2005**, 40, 887.

RED MUD AS A CATALYST FOR THE DECOMPOSITION OF SODIUM BOROHYDRIDE

Fedchenko Anastasiia, Brychenko Iryna, Ivanenko Iryna, Kosogina Iryna
Department of Inorganic Substances Technology, Water Treatment and General Chemical Engineering, National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", 4 building, 37 Peremohy ave., 03056, Kyiv, Ukraine
e-mail: irinaivanenko@hotmail.com

The process of obtaining metallurgical alumina from bauxite by the Bayer method leads to the formation of a significant amount of waste, which includes iron compounds and, in part, aluminum, titanium, calcium and silicon compounds. Due to the prevailing content of a fine fraction of red iron oxide, such waste has the generalized name “red mud”. During the storage of such wastes in specially organized sludge storages due to the influence of seasonal temperature fluctuations, changes in air humidity and wind direction, deflation of the fine fraction of “red mud” occurs, which leads to large-scale air pollution not only within the sanitary protection zone, but also in the surrounding territories, leading to environmental pollution. This situation is relevant for many countries of the world.

The key to solving the problem of deflation and accumulation of red mud is the development of a technology for processing red mud and using it as a secondary metal-containing raw material for the manufacture of various materials. One of the directions of the recycling of red mud is the recovery of pure metals from its composition, but its drawback is the difficulty of the selective extraction of valuable components. Another area is the reuse of red mud as a raw material in the manufacture of binders, which is limited by the permissible limits for the content of foreign components without loss of mechanical characteristics. The main direction of the disposal of red mud is the processing of alumina production wastes into reagents for the purification of water and gas media and this direction is actively developing now. However, the search for new ways to utilize and reuse red mud is still an urgent scientific and practical task.

Well know, the red mud has a rich chemical composition, which represents iron(III) oxide (<50%), aluminum(II) oxide (<15%), titanium(II) oxide (<5%), calcium(II) oxide (<5%) and others. For this reason, it is expected that it will exhibit catalytic activity in the heterogeneous catalytic reactions of the redox type to which the process of sodium borohydride hydrolysis belongs. This reaction is the basis of the borohydride fuel cell operation.

In the presented work the structural-adsorption and catalytic properties of the initial and thermally treated red mud were studied. It was found that in the investigated model reaction, the original red mud shows some activity even at room temperature, and this activity increases under heating of sodium borohydride solution to 40 and 50^{o}C. The red mud after pretreated at 600^{o}C shows more catalytically active in the investigated model reaction.

THE PROCESS OF NICKEL NANOPARTICLE FORMATION IN HYDROPHILIC POLYMER / INORGANIC MATRICES

T.B. Zheltonozhskaya[a], N.M. Permyakova[a], A.S. Fomenko[c], D.O. Klymchuk[b], V.V. Klepko[a], L.N. Grishchenko[c], L.O. Vretik[c]
[a] *Institute of Macromolecular Chemistry, National Academy of Sciences of Ukraine,*
48 Kharkivske Shose, 02160 Kyiv, Ukraine
E-mail: arinafomenko120599@gmail.com
[b] *Institute of Botany, National Academy of Sciences of Ukraine, 2 Tereschenkovskaya St.,*
01601 Kyiv, Ukraine
[c] *Taras Shevchenko National University of Kyiv, Faculty of Chemistry, Department of*
Macromolecular Chemistry, 60 Volodimirska St., 01033 Kyiv, Ukraine

Hydrophilic polymer/inorganic hybrids containing silica nanoparticles and polyacrylamide chains (SiO_2/PAAm) proved to be effective matrices for the *in situ* synthesis of silver nanoparticles, due to which an active and stable biocidal composition with wide functional capabilities is formed in an aqueous solution [1]. A similar approach was used in the present work to obtain small magnetic Ni nanoparticles stabilized in the grafted SiO_2/PAAm hybrids.

The hybrid sample was synthesized by free-radical polymerization of PAAm from the unmodified surface of SiO_2 nanoparticles, and its main parameters (size of inorganic nanoparticles, moisture content, number and length of grafts) were determined using static light scattering, elemental analysis, DTGA and viscometry. The processes of borohydride reduction of the Ni-salt to nanoparticles in hybrid aqueous solutions and pure water were studied depending on the concentration of salt and hybrid using UV-Vis spectroscopy, TEM, and WAXS. The following effects were established: i) an increase in the rate of accumulation and yield of NiNPs with increasing Ni-salt concentration, and ii) a slowdown in the reduction process in hybrid solutions compared to pure water. It was shown that the main structural elements of the obtained nanocomposite are the swollen hybrid particles containing small (~1-7 nm) spherical crystalline NiNPs in the polymer “corona”.

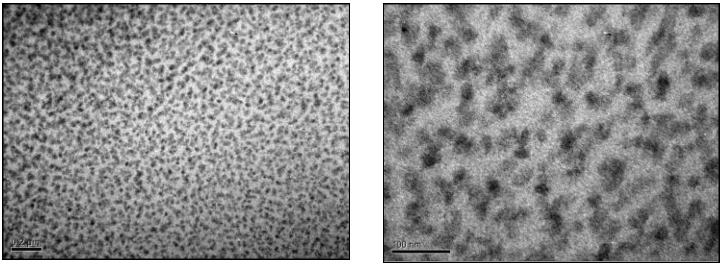


Figure. TEM images of NiNPs formed in SiO_2/PAAm hybrids as matrices.

[1] T.B. Zheltonozhskaya, N.M. Permyakova, T.O. Kondratiuk, T.V. Beregova, V.V. Klepko, B.S. Melnik. Hybrid-stabilized silver nanoparticles and their biological impact on hospital infections, healing wounds, and wheat cultivation, *French-Ukainian J. Chem.*, **2019**,.7, 20-39.

COMPOSITIONAL EFFECT ON THERMOTROPIC PHASE TRANSITIONS IN LONG-CHAIN *n*-ALKANOIC ACIDS BINARY MIXTURES

T.A. Gavrilko[a]*, I.I. Gnatyuk[a], V.I. Styopkin[a], N.D. Shcherban[b], J. Baran[c], M. Drozd[c]
[a]*Institute of Physics, NAS of Ukraine, 46 Nauki Ave., 03028 Kyiv, Ukraine*
[b]*L.V. Pisarzhevsky Institute of Physical Chemistry NAS of Ukraine,*
31 Nauki Ave., 03028 Kyiv, Ukraine
[c]*Włodzimierz Trzebiatowski Institute of Low Temperature and Structure Research, PAS,*
2 Okolna Str., 50-422 Wroclaw, Poland
**Corresponding author: gavrilko@gmail.com*

Long-chain *n*-alkanoic (fatty) acids have been in the focus of intense researches since the beginning of the last century because they are the major components of oils and fats. Lately, an increased interest to these compounds is due to their application in the production of coatings, plastics, as well as phase change materials for energy storage. The utilization of long-chain n-alkanoic acids in the chemical, food and pharmaceutical industries requires a good knowledge of their properties and phase behavior, but the study of the crystal forms of pure fatty acids and especially their binary mixtures still is a challenging task. In the present work, polymorphic phase transitions in solid binary mixtures of stearic, $C_{18}H_{37}OOH$ (SA), and behenic, $C_{22}H_{43}OOH$ (BA) acids, SA_x:BA_{1-x}, with different molar ratios (x=0.5; 0.2; 0.4, and 0.8) were studied using temperature-variable FTIR spectroscopy (Bruker IFS-88, SPECAC variable temperature cell P/N 21.500 with Eurotherm controller 847) in 25-120°C temperature range complemented by DSC measurements (Perkin-Elmer Model 8000) and room-temperature X-ray diffraction (Bruker D8 Advance, $Cu_{K\alpha}$ radiation). To the best of our knowledge, FTIR study of this system had never previously been reported in the literature.

With XRD analysis it was found that the diffraction pattern observed for equimolar SA:BA binary system differs from those of the initial acids, which indicate the formation of a solid solution or a new compound at this concentration. DSC study revealed two solid-solid phase transitions in the SA:BA binary system, that correspond to different intermediate rotator crystalline states, contrary to a single melting transition observed for the initial compounds. Meanwhile, the melting temperature of the binary system significantly decreases compared to the initial acids being close to that of the shorter acid. From the analysis of the temperature-variable FTIR spectra, it was shown that the phase transitions revealed by thermal analysis are associated with an increase of conformational disorder and reorientational motions that contribute to the lattice instabilities in the crystalline mixtures. The results are compared with recently reported [1] full phase diagrams for the SA_x:BA_{1-x} binary systems.

[1] M.C. Costa, M.P. Rolemberg, A.J.A. Meirelles, J.A.P. Coutinho, M.A. Krähenbühl. Thermochim. Acta 496 (2009) 30–37; Chem. Phys. Lipids 157 (2009) 40–50.

DISTRIBUTION INHOMOGENEITY OF NEMATIC 5CB CONFINED TO MOLECULAR SIEVES BY FTIR SPECTROSCOPY AND CARS IMAGING

I. Gnatyuk[a]*, A. Dementjev[b], T. Gavrilko[a], R. Karpicz[b], J. Baran[c], N. Shcherban[d]
[a]*Institute of Physics, NAS of Ukraine, 46 Nauki Ave., 03028 Kiev, Ukraine*
[b] *Center for Physical Sciences and Technology, 3 Sauletekio Ave., Vilnius, LT-10257, Vilnius, Lithuania*
[c]*Institute of Low Temperature and Structure Research, 2 Okolna Str., PAS, Wrocław, Poland*
[d]*Institute of Physical Chemistry NAS of Ukraine, 31 Nauki Ave., 03028 Kyiv, Ukraine*
e-mail: ivan.gnatyuk@gmail.com

The nematic liquid crystal 4-cyano-4'-pentylbiphenyl (5CB) was confined to silica mesoporous molecular sieves with constant composition but different pore size and morphology (Al-MCM-41, KIT-6, and SBA-15). FTIR spectroscopy (Bruker IFS-88) was applied to analyze the amount of loaded 5CB molecules. A home-built CARS microscope with a simple and compact laser (EKSPLA Ltd.) was used to visualize the studied systems. Fourier transform infrared analysis proved that the confined 5CB molecules interact with the pore walls of the molecular sieves via the polar C≡N group. From the analysis of the intensity and peak position of major IR absorption bands, the fractions of 5CB molecules anchored at the pore surface of the MCM-41 molecular sieves with respect to those filling the pores inner space in a bulk-like state has been evaluated. With CARS microscopy, the non-homogenous distribution of liquid crystal's density inside the investigated hosts was found. It was shown that Al-MCM-41 molecular sieves demonstrated the maximum density of the surface species and filling homogeneity, while in SBA-15 the amount of absorbed molecules was less and their density distribution non-homogeneous, and finally KIT-6 mesopores have the poorest adsorption characteristics due to the features of the three-dimensional cubic structure, the larger pore volume and thickness of the walls of the framework. Thus, new possibilities of CARS microscopy for visualization and express analysis of the nematic liquid crystal confined to mesoporous silica-based molecular sieves were shown. The data obtained may be used in such applications as controlled technological separation processes, the development of more effective hosts for targeted drugs delivery, etc.

This work was supported by the National Academy of Sciences of Ukraine under the Ukrainian Governmental Program KPKVK 6541230 "In Support of Priority Research Development", and under the Polish-Ukrainian Scientific Cooperation Program (Project "Structural and optical properties of disordered molecular systems for optoelectronics"), and by the Ministry of Education and Science of Ukraine in the frame of Ukrainian-Lithuanian Scientific Cooperation Program (project No. S-LU-18-6).

ORGANIC BIPOLAR EMITTERS FOR OLEDs AND OXYGEN SENSORS

J. V. Grazulevicius[1], N. Kukhta[1], R. Pashazadeh[1], E. Skuodis[1], A. Tomkeviciene[1], R. Keruckiene[1], J. Simokaitiene[1], M. Cekaviciute[1], Xiaofeng Tan[1], D. Volyniuk[1], K. Ivaniuk[2], P. Stakhira[2]

[1] *Department of Polymer Chemistry and Technology, Kaunas University of Technology, Barsausko 39, LT- 51423 Kaunas, Lithuania.* *e-mail:* *juozas.grazulevicius@ktu.lt*

[2] *Lviv Polytechnic National University, S. Bandera 12, 79013 Lviv, Ukraine*

Organic emitters containing donor and acceptor moieties recently synthesized at the laboratories of the presenting author will be reported.

Derivative of 3-(trifluoromethyl)benzonitrile and 3,3’-bicarbazole was found to exhibit both TADF and exciplex-forming properties [1]. Warm-white OLED based on this material showed external quantum efficiency (EQE) of ca. 20 %.

The derivative of acridan and dicyanobenzene was found to be efficient TADF-emitter exhibiting both thermally activated delayed fluorescence and aggregation induced emission enhancement. Green OLED fabricated using this emitter exhibited maximum current, power efficiency and EQE of 68 cd/m^2, 62 lm/W and 22.5 %, respectively [2].

A series of carbazole-quinoxaline-carbazole derivatives exhibiting TADF and mechanochromic luminescence were synthesized and studied. Green-blue to green-yellow TADF OLEDs fabricated by solution processing demonstrated EQE up to 10.9% and luminance of 16760 cd m^{-2} [3].

By utilization of the derivatives cyanophenyl and ditertbutylcarbazolyl substituted triphenylbenzene with the different substitution pattern as host and guest of the emissive layer, deep-blue OLED based on triplet-triplet annihilation with EQE of 14.1% as fabricated [4].

Derivatives of thianthrene and benzophenone exhibited room-temperature phosphorescence and demonstrated oxygen sensing ability [5]

Derivatives of benzotrifluoride and 3,7-di-tert-butyl-phenothiazine were synthesized and studied as active materials for optical sensors of oxygen [6]. Oxygen sensing abilities of the compounds were tested. Practically the same phosphorescence intensity after several cycles of evacuation and refilling was recorded for one compound.

Acknowledgment. This research was funded by European Union’s Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie Research and Innovation Staff Exchange (RISE) scheme (grant agreement No 823720).

[1] G. Grybauskaite-Kaminskiene G et al., J. Mater. Chem. C, **2019**, 6, 1543-1550.

[2] E. Skuodis et. al., Org. Electron., **2018**, 63, 29-40.

[3] R. Pashazadeh et. al., J. Phys. Chem. Lett., **2018**, 9, 1172- 1177.

[4] N. Kukhta et al., J. Phys. Chem. Lett., **2017**, 8, 6199-6205.

[5] A. Tomkeviciene et al, Dyes. Pigm., **2019**, 170, UNSP 107605

[6] R. Keruckiene, submitted to Sens. Actuators B, **2020**.

SYNTHESIS AND PROPERTIES OF D-A-D-TYPE ORGANIC SEMICONDUCTING MATERIALS BASED ON A FLUORENONE MOIETY

Dalius Gudeika[a], Oleksandr Bezvikonnyi[a], Dmytro Volyniuk[a], Juozas Vidas Grazulevicius[a]
[a] *Department of Polymer Chemistry and Technology, Kaunas University of Technology,Radvilenu pl. 19, LT-50254, Kaunas, Lithuania.*
e-mail: *gudeika.dalius@gmail.com*

Organic blue light emitting materials have attracted much attention because of their applications in flat-panel displays and solid-state lighting [1]. In this work a series of new fluorenone-based compounds have been synthesized and characterized using ^{1}H NMR, ^{13}C NMR, FT-IR spectroscopy, mass spectrometry and elemental analysis. 2,7-Bis(3,6-di-*tert*-butyl-9*H*-carbazolyl)-9-fuorenone, 2,7-bis(phenothiazinyl)-9-fuorenone, 2,7-bis(9,9-dimethyl-9,10-dihydroacridinyl)-9-fuorenone and 2,7-bis(phenoxazinyl)-9-fuorenone were synthesized by Buchwald-Hartwig coupling method. The compounds thermal, electrochemical and optical properties have been investigated. The synthesized compounds showed relatively high thermal stabilities: 5% weight loss starts from 365 °C.

Photophysical properties of the solutions in toluene of the synthesized compounds were studied. The absorption maximum range from 467 to 506 nm, while photoluminescence maximum range were distributed between 596 and 707 nm. The synthesized compounds ionization potentials were ranged from 5.18 to 5.47 eV.

Acknowledgement

This project has received funding from the Research Council of Lithuania (LMTLT), agreement No [S-LU-20-3].

References

[1] S. O. Jeon, S. E. Jang, H. S. Son, J. Y. Lee. Adv. Mater. **23**, 1436-1441, (2011).

THERMAL HYSTERESIS IN SPIN-CROSSOVER NANOCRYSTALS WITH (ANTI)FERROMAGNETIC SURFACE

Iu. Gudyma[a], A. Maksymov[b]
[a] *Physical, Technical and Computer Sciences Institute, Yuriy Fedcovich Chernivtsi National University, Kotsyubynsky 2, Chernivtsi 58012, Ukraine*
e-mail: yugudyma@gmail.com
[b] *Marian Smoluchowski Institute of Physics, Jagiellonian University, Lojasiewicza 11, Krakow 30-348, Poland*
e-mail: maxyartur@gmail.com

The pseudo-octahedral transition metal coordination complexes may undergo spin-crossover (SCO) transitions from a diamagnetic low-spin (LS) to a paramagnetic high-spin (HS) states under the effect of a weak external perturbation (temperature, pressure, light, magnetic or electrical field). The spin states of a SCO compound demonstrate various magnetic, optical, structural and electrical properties. The molecules in HS state are characterized by larger volume and higher effective degeneracy than the ones in the LS state. The size difference between the HS and LS molecules provokes local elastic distortions that lead to an effective long-range elastic interaction.

In this work we have focused on the thermal hysteresis exhibited by spin-crossover nanocrystals with inhomogeneous interactions changing from the surface to the bulk of the lattice. We have considered the model of 3D nanocrystal with ferromagnetic and antiferromagnetic coupling of the sites on the surface. Phenomenologically, the magnetization properties in molecular spin-crossover nanoparticles with mentioned types of interactions can be modeled by the Ising-like Hamiltonian of the following form [1,2]

$$H = -h_0\sum_i s_i - \sum_{ij}^{b} J_{ij}^{b} s_i s_j - \sum_{<ij>}^{s} J_{ij}^{s} s_i s_j - \sum_{<ij>}^{b-s} J_{ij}^{b-s} s_i s_j, \qquad (1)$$

where h_0 is external effective field, s_i is pseudospin operator which has two eigenvalues ± 1, corresponding to the HS and LS states of respective i-th molecule, J_{ij}^{α} is the intersites short-range coupling constants with $\alpha = s, b, b-s,$ which correspond to occupied pairs of bulk sites, surface sites and bulk-surface sites respectively.

By using Monte Carlo numerical simulations the properties of spin-crossover 3D nanocrystals have been analyzed in terms of cooperativity accounting its changing from the surface of nanocrystal to the bulk of lattice. We have shown that the nature of cooperativity for sites on the surface drastically impacts the completeness of phase transition. In the system with antiferromagnetic surface the temperature transition curves show a premature saturation with smaller magnetization value for HS state and greater one for LS configuration. The obtained numerical results show very good agreement with the experimental studies.

[1] Iu. Gudyma, A. Maksymov, Appl. Surf. Sci., **2017**, 407, 93-98.
[2] Iu. Gudyma, A. Maksymov, Appl. Surf. Sci., **2019**, 483 779-784.

REFINEMENT OF THE PHASE DIAGRAM OF THE Bi-Se SYSTEM AND THERMODYNAMIC PROPERTIES OF THE BISMUTH SELENIDES

[a]Zeynalova G.S., [a]Mammadova A.T., [b]Aghazade A.I.,[b]Imamaliyeva S.Z., [b]Babanly M.B.
[a]*Ganja State University, 187, Khatai ave., AZ-2000, Azerbaijan*
[b]*Institute of Catalysis and Inorganic Chemistry, ANAS, 113, H.Javid, AZ-1143, Azerbaijan*
e-mail: babanlymb@gmail.com

Bi_2Se_3 and other bismuth selenides have a tetradimite-like layered structure and are polyfunctional materials with thermoelectric, topological insulator and other properties [1-3].

However, a number of bismuth selenides were not reflected in the phase diagram of this system. This paper presents the results of the refinement of the phase diagram of the Bi-Se system and studying the thermodynamic properties of bismuth selenides.

Alloys of compositions 40-60 at% Se were obtained by melting of the stoichiometric amounts of elementary components in vacuumed quartz ampoules at 750^0C with subsequent quenching in cold water and annealing at 450 ^{0}C for 800-1000 h.

The studies were carried out using the methods DTA (NETZSCH 404 F1 Pegasus differential scanning calorimeter), XRD (Bruker D8 ADVANCE powder diffractometer utilizing CuK_αradiation within 2θ = 10 to 70°) and EMF measurements of the concentration chains of the type

$$(-)\ Bi\ (solid)\ /\ ionic\ liquid,\ Bi^{3+}\ /\ (Bi\ in\ alloy)\ (solid)\ (+) \qquad (1)$$

in the 25-170^0C temperature range. The technique for assembling an electrochemical cell and conducting experiments is described in detail in [4].

Based on the obtained data, it was shown that in addition to Bi_2Se_3 with congruent melting at 705 ^{0}C, the following compounds with incongruent meltings by peritectic reactions: Bi_3Se_4 (617^0C), Bi_8Se_9 (608^0C), BiSe (593^0C), Bi_8Se_7 (580^0C), Bi_4Se_3 (556^0C), Bi_3Se_2 (469^0C) are formed in the system The types and parameters of crystal structures of specified intermediate compounds are determined.

From the data of (1) type cells, the linear equation of the type $E = a + bT$ for various phase areas are obtained, based on which partial thermodynamic functions of bismuth in alloys were calculated. Based on the solid phase equilibria diagram the potential-forming reactions for bismuth selenides were established, and their standard Gibbs energy of formation and enthalpy of formation, as well as the standard entropies, were calculated. For Bi_2Se_3, the obtained values are in good agreement with the literature data, while for the remain compounds they were determined for the first time.

The work has been carried out within the framework of the international joint research laboratory "Advanced Materials for Spintronics and Quantum Computing" (AMSQC) established between Institute of Catalysis and Inorganic Chemistry of ANAS (Azerbaijan) and Donostia International Physics Center (Basque Country, Spain) and partially funded by a grant EİF/MQM/Elm-Tehsil-1-2016-1(26)-71/01/4-M-33.

[1] Hogan C., Holtgrewe K. et al., *ACS Nano*, **2019**, 13(9), 10481.
[2] Flammini R., Colonna S. et al. *Nanotechnology*, **2018**, 29(6), 065704.
[3] Shevel'kov A.V., *Russ. Chem. Rev*, **2008, 77**, 1.
[4] Imamaliyeva S.Z., Musayeva S.S. et al. *Thermochimica Acta*, **2019**, 679, 178319.

CALCIUM CARBONATE IN THE FORM OF SPHERICAL PARTICLES: SYNTHESIS AND PROPERTIES

N.V. Guzenko, O.L. Gabchak, O.I. Oranska
Chuiko Institute of Surface Chemistry, NAS of Ukraine, 17 General Naumov Str., Kyiv 03164, Ukraine.
e-mail: guznataliia@gmail.com

Calcium carbonate consisting of particles, the crystalline phase, morphology, size and particle size distribution of which are strictly controlled and can be changed in accordance with specified requirements, today is promising in the manufacture of paper, paint, rubber, plastics, binders, cosmetic products as well as in biological applications, including drug delivery. The task of synthesis of porous spherical calcium carbonate particles with a monodisperse particle size distribution can be solved only with careful selection of experimental conditions and is determined by many factors: concentration of initial solutions, introduction speed of the second reagent, mixing intensity and time, use of additional structure-forming substances and so on [1, 2].

In the study the structure of $CaCO_3$ particles, synthesized from high concentrated Ca^{2+} and CO_3^{2-} solutions, was characterized by microscopy, low-temperature adsorption of nitrogen and argon, X-ray diffraction analysis and Infra-red spectroscopy. It was shown that at rapid addition and low intensity of reagent solutions mixing, large (7.8–11.4 μm) non-porous (S_{BET} = 0.40–0.48 m^2/g) calcium carbonate particles can be obtained, the crystalline modifications of which were represented exclusively by calcite.

Porous spherical calcium carbonate particles with monodisperse distribution of diameters in the range of 3.6-4.5 μm can be obtained at low speeds of reagent introduction and uniform mixing with intensity in the range of 500-1000 rpm. Uniform, sufficiently intensive mixing does not contribute to the growth of large crystals, on the contrary, a large number of small crystals of vaterite and calcite are formed, which under these conditions aggregate into fairly uniform micron-sized spherulites. The samples of these micrometer-sized aggregates had a pore volume of 0.1 cm^3/g, a pore width of about 20-30 nm, and a specific surface area of about 13-17 m^2/g.

With an increase in the intensity of mixing of the initial solutions to 2000 rpm, the force of external influence probably exceeds considerably the forces of interparticle interaction, and aggregation of crystals does not occur. So, in this case particles with the absence of clear micron-sized structures with a high content of calcite were obtained; the value of the specific surface area for them was about 3-6 m^2/g.

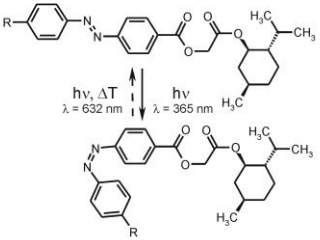
[1] M. Abebe N. Hedin, Z. Bacsik, *Crystal Growth Design*, **2015**, 15(8), 3609–3616.
[2] S. Biradar, P. Ravichandran, R. Gopikrishnan et al, *Journal of Nanoscience and Nanotechnology*, **2011**, 11(8), 6868-6874.

SYNTHESIS AND CHARACTERIZATION OF PHOTOSENSITIVE CHIRAL DOPANT FOR APPLICATIONS IN LIQUID CRYSTALS

V. O. Chornous [a], M. V. Vovk [b], Yu. V. Dmytriv [c,d], A. V. Rudnichenko [c,e],
M. V. Skorobahatko [d], L. N. Lisetski [f], I. A. Gvozdovskyy [g]
[a] *Bukovinian State Medical University, Teatralnaya Square 2, Chernivtsi, 58002, Ukraine*
[b] *Institute of Organic Chemistry, NAS of Ukraine, Murmanska Str. 5, Kyiv, 02660, Ukraine*
[c] *Enamine Ltd, Chervonotkatska Str 78, Kyiv, 02094, Ukraine*
[d] *National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", Prospekt Peremohy 37, Kyiv, 03056, Ukraine*
[e] *National Taras Shevchenko University, Volodymyrska Str. 64, Kyiv, 01033, Ukraine*
[f] *Institute for Scintillation Materials of STC "Institute for Single Crystals", NAS of Ukraine, Prospekt Nauky 60, Kharkiv, 61072, Ukraine*
[g] *Institute of Physics, NAS of Ukraine, Prospekt Nauki 46, Kyiv, 03028, Ukraine*
e-mail: igvozd@gmail.com

It is known that the addition of chiral dopants (ChDs) to nematics leads to the formation of cholesteric liquid crystals (CLCs), which possess helical structure with the director ***n*** twisted uniformly along the helical axis. In spite of the fact that nowadays CLCs are generally well studied, the interest to synthesis of various ChDs with controlled characteristics and their detailed investigation remain important goals both for science and applications.

Here, we present the newly synthesized ChD-3501, consisting of azo- and aliphatic fragment with a chiral center (Figure 1). To introduce the chiral center, we used *l*-menthol in a way similar to the previously described [1]. The spectral kinetics of ethanol solution of ChD-3501 was studied under UV/VIS irradiation and temperature. It was found that ChD-3501 could undergo reversible *trans-cis* isomerization under UV/VIS irradiation. In addition, it has been found that the storage of ChD-3501 *cis*-isomer at certain constant temperature also leads to the reversible isomerization.



The concentration and irradiation-time dependences of the helical pitch of the chiral mixture of ChD-3501 dissolved in the nematic E7 were studied. The effects of UV/VIS on the unwinding and winding of the cholesteric helix were determined both for the wedge-like LC cell with tangential anchoring and parallel LC cell with homeotropic anchoring. In addition, the reversible process of winding of the cholesteric helix when stored in LC cells at the temperature of 80° C was also realized.

[1] S. N. Yarmolenko, L. A. Kutulya, V. V. Vaschenko, L. V. Chepeleva. Photosensitive chiral dopants with high twisting power. *Liq Cryst*, **1994**, 16, 877–882.

UTILIZATION OF A NEW DESIGNED ELECTROMECHANICAL REACTOR FOR HEAVY METALS REMOVAL IN AN INDUSTRIAL WASTEWATER TREATMENT PROCESS USING ORGANIC AND INORGANIC MATERIALS

Amir Hajiali
University Politehnica of Bucharest, Splaiul Independentei St., Bucharest 060042, Romania
e-mail: a.hajiali.env@gmail.com

A lot of effort have been done in mixing tanks regarding functional mixers in wastewater treatment processes, considering the power consumption, mix quality, mixing time and the initial and current costs. For a blending process, reservoirs with different geometric shapes and different butterflies are used. Due to the complexity of the mixing process, research in this subject is still of particular importance and emphasis on empirical studies. Changing the design of an existing agitator to improve efficiency, like the design of a new mixing system, requires careful studying [1]. In reactor construction, several parameters are effective, one of which is a mechanical mixers. Important points to be considered in the mixing process are the choice of a suitable permit for less power consumption and shorter mixing times, as well as eliminating or reducing the effect of vortices.

In this research, biological absorbents of ferns was prepared and then removal of iron and zinc metals was investigated by these two adsorbents. It should be noted that effective parameters on removal such as pH, time, pollutant concentration and adsorption concentration were investigated and then tested with optimal amounts of actual wastewater. The results of this section were used in the semi-industrial section.

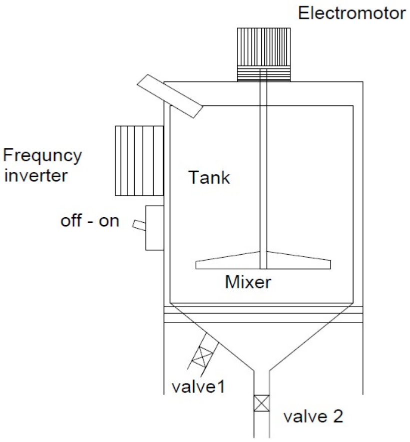


Figure 1: Schematic of batch pilot

In this project, for the initial experiments, the Jarring test device was used as a discontinuous mixer reactor for the mixing of effluent and adsorbent in the laboratory (Section I). The reason for this choice is to create conditions that are almost identical to those of a continuously stirred reactor. In the second stage, the reactor based on the most efficiency was designed and constructed on a semi-industrial scale and the removal rate of iron and zinc contaminated metals was achieved in optimal conditions from the first stage (Section II).

After determining the optimal conditions for absorbent performance on a laboratory scale, the removal of two zinc and iron metals by ferns and dry sludge adsorbents on the industrial scale was investigated for the actual treatment and the synthetic wastewater treatment.

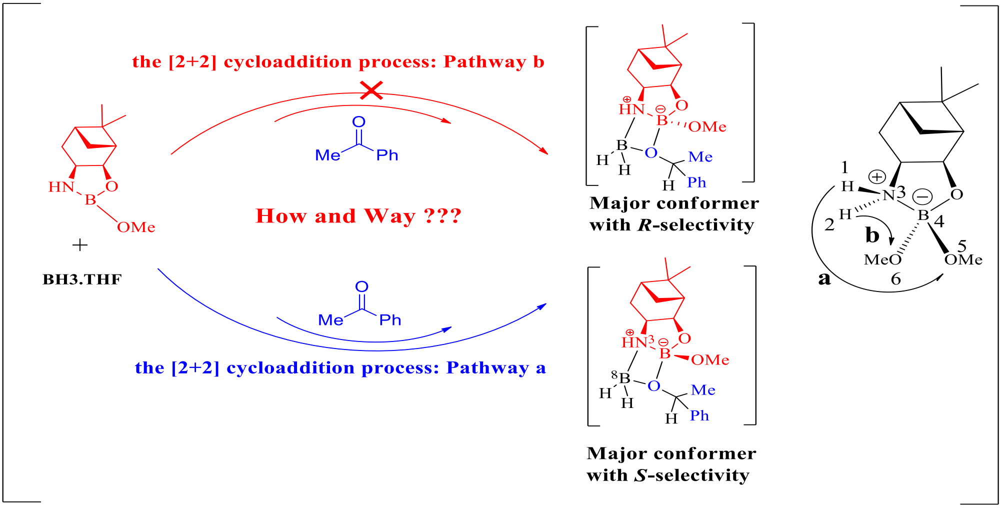
Pilot components according to the design and studies carried out and the cost of conducting it has been accomplished. In figure 1 the schematic of the batch pilot can be seen.

[1] RF Goncalve, VL de Araujo, CAL Chernicharo, ‘’Association of a UASB Reactor and a Submerged Aerated Bio Filter for Domestic Sewage Treatment’’, *Water Science Technology*, **1998**; 38(8/9):189-199.

UNDERSTANDING THE ORIGIN OF THE CHANGE OF THE ENANTIOSELECTIVITY IN THE CYCLOADDITION STEP IN THE THE REACTION MECHANISM OF ENANTIOSELECTIVE REDUCTION OF KETONES WITH BORANE CATALYZED BY A *B*-METHOXY OXAZABOROLIDINE CATALYST DERIVED FROM (–)-Β-PINENE: A DFT STUDY

Hichem Sadrik Kettouche
Laboratoire des produits naturels d’origine végétale et de synthèse organique, Département de Chimie, Université Mentouri de Constantine. Route Aine El Bey, 25000 Constantine, Algérie
E mail: kettouchehichem@gmail.com

A theoretical study has been conducted by means of the functional theory method (DFT) to more understanding the origin of the change of the enantioselectivity during the formation of four-membered ring (B(8)-N(3)-B(4)-O(7)) via the [2 + 2] cycloaddition reaction step in the reaction mechanism of Enantioselective Reduction of ketones with borane catalyzed by a *B*-Methoxy Oxazaborolidine Catalyst Derived from (–)-β-Pinene. It has been proven that this cycloaddition step involves four structures of transition state such as **TS5a(*S*), TS5a(*R*)**, **TS5b(*S*)** and **TS5b(*R*)**. They are in one-to-one correspondence to the four conformers **M6a(*S*)**, **M6a(*R*), M6b(*S*)** and **M6b(*R*)** (**a** mode denotes the implication of the kind **a** of oxazaborolidine, while the **b** one refers to the implication of kind **b.** A comparative assessment between the B3LY, M06 and MPWB1K functional has been performed which, shows that while the B3LYP functional fails to find the right enantioselectivity In the cycloaddition step and the M06 is not the appropriate one in therms of thermodynamic controlled the CA reaction, the MPWB1K one proves to be the relevant one for both kinetic and thermodynamically controlled the formed four-membered ring (B-N-B-O) via the [2 + 2] cycloaddition reaction through the coordination between the carbonyl oxygen of aromatic and the B site to produce the right reaction pathway that we have been optimized completely All the structures using the functional MPWB1K /6-31G (d,p). Inclusion of solvent effects slightly increases the activation energy and decreases the exothermic character of the CA reaction. The electron localization function (ELF) reveals that the formation of the B–N and O–B bonds occurs via non-concerted two-stage one-step mechanism. topological analysis Non-covalent interaction analysis of the four computed transition states associated with formation of four-membered ring (B-O-B-N) via the [2 + 2] cycloaddition reaction discloses that **TS3a(S)** is the stable conformation with respect to **TS3a(R)**, which is aligned withe S-selecivity obtained along the whole pathway of the reaction mechanism.



Réference

Hichem Sadrik Kettouche. A DFT Study on the reaction mechanism of Enantioselective Reduction of ketones with borane catalyzed by a *B*-Methoxy Oxazaborolidine Catalyst Derived from (–)-β-Pinene. *Journal of Molecular Modeling*, **26,** 27 (2020)

SURFACE MORPHOLOGY OF NANOSTRUCTURED GAS SENSORS BASED ON METAL-POLYMER COMPOUNDS

D.O. Harbuz[a,b], A.P. Pospelov[a], M.D. Romanov[b], P.V. Mateychenko[c], A.P. Konotop[b], V.A. Gudimenko[b], G.V. Kamarchuk[b]
[a]*National Technical University "Kharkiv Polytechnic Institute", 2 Kyrpychov Str., Kharkiv, 61002, Ukraine*
[b]*B. Verkin Institute for Low Temperature Physics & Engineering, 47 Nauky Ave., Kharkiv, 61103, Ukraine*
[c]*Institute for Single Crystals, National Academy of Sciences of the Ukraine, 60 Nauky Ave., Kharkiv, 61000, Ukraine*
e-mail: Zeyxes@gmail.com

In recent years, highly sensitive gas sensors have become increasingly popular. The field of their application varied widely, from medical sensors that could detect oncological diseases by the human breath [1], to sensors that could detect the methane, without which modern mining would not be possible.

In the present study, we create and investigate conductive gas sensors based on the point-contact gas sensitivity effect. Samples are obtained by combined electrochemical deposition. The TCNQ compound was used as a sensitive material for those devices. In our case, the Yanson point contact serves as simplest gas sensor which is formed between two crystals of Cu-TCNQ. Each gas sensor is a complex multistructure and includes a several hundred point contacts. Earlier we demonstrated the wide possibilities of such sensors in studies aimed at the diagnosis and differentiation various strains of the *Helicobacter Pylori* infection [2].

The features of Cu-TCNQ compounds include the variety of morphologies of their crystals, as well as their polymorphic nature. This study was aimed to investigate the dependence between the deposition conditions and the resulting surface morphology and their correlation with electrophysical properties of gas sensors based on Cu-TCNQ compounds.

The results of our research have allowed us to clarify the influence of deposition parameters on the structure of the resulting samples. During the work, the optimal deposition parameters were investigated and an automatic laboratory deposition device was developed, which made it possible to obtain a large number of gas sensors in a short time. The data obtained bring closer the introduction of sensors of this type into widespread use.

This work was partly supported by the NATO SPS Programme (Ref: SPS 985481).

[1] Li, W., Liu, H., Xie, D. et al. Lung Cancer Screening Based on Type-different Sensor Arrays. *Sci Rep 7*., **2017**, 1969.

[2] E. Kushch, N. Korenev, L. Kamarchuk. tt al.On the importance of developing a new generation of breath tests for Helicobacter pylori detection, *J. Breath Res*., **2015**, 9(4), 047111.

COBALT-IRON SPINEL / REDUCED GRAPHENE OXIDE COMPOSITE MATERIAL FOR SUPERCAPACITOR APPLICATIONS

Myroslava Hodlevska, Ruslan Zapukhlyak, Volodymyra Boychuk,
Volodymyr Kotsyubynsky, Khrystyna Bandura, Andrii Kachmar, Mykola Hodlevskyi
Vasyl Stefanyk Precarpathian National University,
57 Shevchenko str., Ivano-Frankivsk, 76018 Ukraine
e-mail: kotsuybynsky@gmail.com

The use of composite electrode for hybrid supercapacitors based on spinels and carbon materials allows both electronic conductivity increasing and high specific surface area preserving that results in high redox performance.

Ultrafine cobalt-iron spinel (CIS) was synthesized by hydrothermal route using aqueous solutions of $CoCl_2{\cdot}6H_2O$ and $FeCl_3{\cdot}6H_2O$ (metal molar ratio of 1:2) as precursors, urea as a chelating agent and NH_4F as nanoscale pore forming agent. The synthesis of composite material was done in the same way except for the addition of graphene oxide colloidal solution prepared by Hummers method. The predicted mass ratio of oxide and graphene components is 2:1. The obtained samples was marked as CIS/rGO sample. CIS and CIS/rGO samples were additionally annealed in the temperature range of 200-700 °C in argon atmosphere. According to XRD results the samples of both series are amorphous up to 600 °C. The broadened reflexes in the XRD patterns for samples annealed at 600 and 700 °C correspond to diffraction peaks that are characteristic for disordered spinel structures (JCPDS #22-1086). XRD patterns of composite sample are characterized by the increasing of relative intensity in the angle range of 20-30° that is caused by rGO component presence. The decrease in peak broadening for CIS/rGO pattern indicates the increasing of average particle sizes for carbon-containing material. Mossbauer spectroscopy (^{57}Co (Cr) source, α-Fe calibration) was used to investigate the changes in magnetic and structural arrangement during thermal treatment. The superparamagnetic state of the synthesized material is observed up to annealing temperature of 400 °C (CIS-400 sample). The transition to magnetic ordering continues up to 600°C. The Mossbauer spectra of CIS-700 correspond to monophase spinel structure while CIS/rGO-700 sample contains the α-Fe_2O_3 phase. The Mossbauer spectra of CIS-400 and CIS/rGO-700 at 85 K demonstrate the full transition to magnetically ordered state so the formation of hematite phase occurs at 600 °C.

The electrochemical properties of the obtained materials were analyzed using halvanostatic cycling (three-electrode cell, 1 M aqueous KOH electrolyte). The anodic peak at about 0 V for CIS electrodes (Fig. 1) can be explained by Fe(II)↔Fe (III) redox scheme when wide cathodic peak at about 0.3 V corresponds to Co (II)↔ Co (III) reversible reduction / oxidation process. The maximal specific capacitance values of CIS-400 and CIS/rGO-400 materials are about 40 and 75 F/g, respectively.

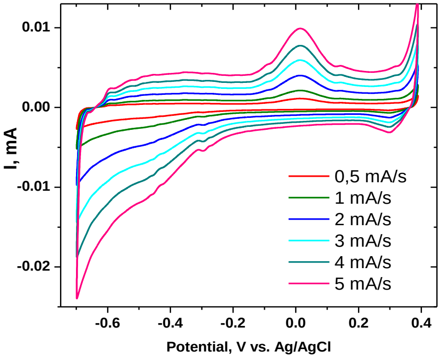


Fig. 1. CVA curves of CIS-400 sample.

DIELECTRIC AND MAGNETIC PROPERTIES OF $KTaO_3$:Li,Co CERAMICS

S. V. Lemishko[a], O. O. Andriiko[b], M. M. Prokopiv[c], M. Trepachko[d], I. S. Golovina[a,e]
[a] *V. Lashkaryov Institute of Semiconductor Physics, National Academy of Sciences of Ukraine, pr. Nauky 45, 03028 Kyiv, Ukraine*
E-mail: sleeper1986@ukr.net
[b] *National Technical University of Ukraine “KPI’”, pr. Peremogy 37, 03056 Kyiv, Ukraine*
[c] *V. Bakul Institute for Superhard Materials, NAS of Ukraine, str. Avtozavodska 2, 04074 Kyiv, Ukraine*
[d] *Institute of Physics, NAS of Ukraine, pr. Nauky 46, Kyiv, Ukraine*
[e] *Drexel University, 3141 Chestnut Street, Philadelphia, PA 19104, USA*

A quantum paraelectric $KTaO_3$ is of interest due to a low value of dielectric losses, 10^{-4}, and high dielectric constant which increases up to 4000 at T=4.2 K. Thanks to its unique properties, $KTaO_3$ has already exploited in EPR spectroscopy [1]. To expand the scope of applications, approaches that may affect the properties of the material are applied.

In this work, we co-dope $KTaO_3$ with Li and Co, and synthesize the material using two technologies that allow to obtain crystals of various sizes. Solid-phase synthesis was used to obtain ~200-nm crystals (KLCTO I), and a technology based on the oxidation of metallic Ta in molten KNO_3 was used to obtain ~80-nm crystals (KLCTO II) [2]. $KTaO_3$ co-doped with 4 mol.% Li and 4 mol.% Co exhibits a relaxor ferroelectric behavior and cluster magnetism. From temperature dependent dielectric data collected at a number of frequencies within interval 1 Hz - 1 MHz, the relaxation characteristics of Li^+ and Co^{2+} ions were determined. The characteristic frequency dispersion obeys the Vogel-Fulcher (VF) law with parameters: $E_a = 0.0167$ eV, $T_{VF} = 22$ K, $\nu_0 = 10^7$ Hz. The Co^{2+} ions relaxation characteristics: activation energy E_a=0.370 eV and 0.399 eV, characteristic frequency $\nu_0 = 8.08*10^{12}$ and $6.57*10^{12}$ Hz for KLCTO I and KLCTO II, respectively. The analysis of temperature dependent magnetic hysteresis loops indicates a higher saturation magnetization, $4*10^{-3}$ and 10^{-2} Am^2/kg, in KLCTO II compared to $2.3*10^{-3}$ and $3.6*10^{-3}$ Am^2/kg in KLTCO I, at T= 290 K and 110 K, respectively. With increasing temperature, a saturation magnetization decreases, while the average size of magnetic clusters increases in both samples (~2100, ~3100 Co atoms per cluster at 110 K and ~3300, ~5600 Co atoms/cluster at 290 K for KLCTO I and KLCTO II, respectively). The latter can be explained by that smaller clusters are destroyed first.

[1] Golovina I. S., Geifman I. N., Rodionov Ye. V. Dielectric resonators for EPR spectroscopy. - Kiev. Institute of Semiconductor Physics of NAS of Ukraine. - 2015.- 158 p.

[2] Andriiko O. O., Kovalenko I. V., Chernenko L. V., Khainakov S. A., Golovina I. S., Geifman I. N. The synthesis of nanosized potassium metatantalate in molten nitrate environment, *Naukovi visti NTUU “KPI”*, **2008**, 1(57), 117-122.

NEW RECORDING MEDIA FOR HOLOGRAPHY BASED ON AZO-DYES OF SUDAN SERIES

Valeriia Ovdenko, Dmitry Vyshnevsky, Nikolay Davidenko, Valeriy Pavlov
Taras Shevchenko National University of Kyiv, 60 Volodymyrska St., Kyiv 01033, Ukraine.
e-mail: valeryovdenko@gmail.com

Materials containing azo chromophore derivatives are potentially suitable for many applications such as optical data storage, holography, optical switching, non-linear optics, solid-state laser. The photoinduced surface deformations in azo-containing thin films are determined by the incident light polarization (perpendicular or paralell) and its intensity. The driving mechanism of the surface grating formation is the cyclic photoindused trans-to-cis isomerization of the azobenzene molecules. The main purpose of this work consists in the study of structure and number of photoactive -N=N- bridges effect on diffraction efficiency of recording media based on PMMA and Sudan series azo dyes. For these purposes, Sudan 1, Sudan 3 and Sudan 4 dyes were selected as a model structures.

The kinetics of the grating growth in the three azo dye/PMMA media under various states of the polarized light has been studied.

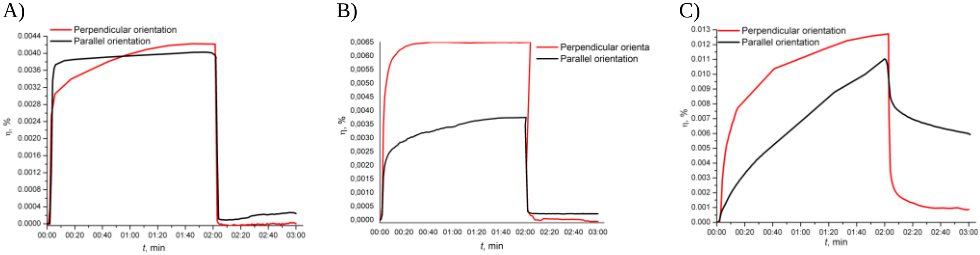


Figure 1. The diffraction efficiency changes in Sudan1/PMMA (A), Sudan3/PMMA (B) and Sudan4/PMMA (C) films for parallel and perpendicular data beam polarization

The diffraction efficiency of the Sudan 1 dye, containing one photoactive group, was expectedly lower than in Sudan 3, which consists of two azobenzene fragments. Both systems were characterized by a sharp increase of diffraction efficiency during recording with further sharp decrease after shuttering the object beam. The introduction of the methyl groups in the ortho-positions to both azo fragments into the structure of dye (Sudan 4) leads to edge smoothing of diffraction efficiency curve.

NEW PHASES OF VARIABLE COMPOSITION BASED ON FAMATINITE MINERAL - POTENTIAL ENVIRONMENTAL FRIENDLY THERMOELECTRIC MATERIALS

[a]Ismailova E.N., [a]Mashadiyeva L.F., [b]Shevelkov A.V, [a]Bakhtiyarly I.B., [a]Babanly M.B.
[a]*Institute of Catalysis and Inorganic Chemistry, ANAS,113, H.Javid, AZ-1143, Azerbaijan*
[b]*Moscow State University, Leninskiye Gory, Moscow, 119899, Russia*
e-mail: babanlymb@gmail.com

Ternary copper and silver chalcogenides are of great interest for many years due to the manifestation of photovoltaic, thermoelectric, optical, and others functional properties, as well as mixed electronic-ionic conductivity [1]. In particular, synthetic analogues of copper minerals: chalcostibite ($CuSbS_2$), skinnerite (Cu_3SbS_3), famatinite (Cu_3SbS_4), etc. are of great practical interest due the possibility of developing new environmentally friendly thermoelectric materials on their basis [2, 3]. One of the ways to optimize the functional properties of known compounds is obtaining solid solutions on their basis. Considering the above, the solubility based on the Cu_3SbS_4 compound in the Cu_3SbS_4-GeS_2 (A) and Cu_3SbS_4-SnS_2 (B) systems is studied.

The starting compounds of the studied systems were prepared by melting the elemental constituents of high purity (99.999%) in evacuated (up to 10^{-2} Pa), and sealed quartz ampoules at temperatures up to 50 ° above the melting points in two-zone mode. Alloys of the studied systems, each weighing 0.5 g, were obtained by fusion of stoichiometric amounts of pre-synthesized and identified starting compounds under vacuum at 700 °C with further annealing at 450 °C for 500 h. The alloys were investigated by means of DTA, XRD, and SEM.

A joint analysis of the experimental data showed that the solubility based on the Cu_3SbS_4 compound is not less than 20 mol% GeS_2 in system A, and not less than 30 mol% SnS_2 in system B. In the outside the regions of homogeneity, a complex picture of phase equilibria for both studied systems is observed. Both studied systems are unstable below solidus.

Thus, despite the difference in the crystal lattices of the starting compounds in the both studied systems, a rather wide solubility region based on the compound Cu_3SbS_4 is observed. Apparently, this is due to the fact that in the replacement of Sb^{5+} ions by Ge^{4+} (Sn^{4+}) ions, their charge difference is compensated by the transition of a part of Cu^{+} ions to the Cu^{2+} state.

This work was supported by the Science Development Foundation under the President of the Republic of Azerbaijan – Grant № EİF-BGM-4-RFTF-1/2017-21/11/4-M-12.

[1] Applications of Chalcogenides: S, Se, and Te. Ed. Ahluwalia G.K, 2016, Cham.: Springer, 461 p.
[2] Suekun K.; Takabatake T., *Apl. Mater*., **2016**, 4, 104503.
[3] Nasonova D. I., Verchenko V. Y., et al., *Chemistry of Materials*, **2016**, 28(18), 6621–6627.

HIGH-ε CERAMICS FOR EPR RESONATOR INSERT

S. V. Lemishko[1], V. O. Yukhymchuk[1], I. P. Vorona[1], I. S. Golovina[1,2],
S. O. Solopan[3], A. G. Belous[3]
*[1]V. Lashkaryov Institute of Semiconductor Physics, National Academy of Sciences of Ukraine,
pr. Nauky 45, 03028 Kyiv, Ukraine*
[2]Drexel University, 3141 Chestnut Street, Philadelphia, PA 19104, USA
*[3]V.I. Vernadskii Institute of General and Inorganic Chemistry of the NAS of Ukraine, Kyiv
Ukraine*
E-mail: sleeper1986@ukr.net

In recent years, much of the research has focused on the analysis of the properties of small objects, such as thin films with an active layer thickness of 10-100 nm and nanocomposite materials, with particles size of 1-100 nm. In many cases, such objects cannot be obtained in an amount sufficient for the study by traditional methods, or their properties change substantially in the case of increasing size. All this makes the task of increasing the sensitivity of traditional research methods extremely important.

One of the methods of increasing the sensitivity of EPR spectrometers is to use so-called dielectric resonators (DR) or dielectric inserts (DI) made of materials with a high dielectric constant ε [1]. The amplification of the EPR signal by DI is due to the redistribution and enhancement of microwave power in the small volume of the high-ε resonator, where the test sample is placed.

Thus, the purpose of this study was to calculate the DI resonance dimensions and determine the distribution of the magnetic and electrical components of a standing electromagnetic wave in the metallic cavity when there is an insert made of a high-ε dielectric material in the resonator, in order to establish the optimal parameters of the DI. The modeling computer calculations were made using Ansoft HFSS simulation package. It was found that the cylindrical shape of the DI is optimal, with the following dimensions: outer diameter ~5 mm, inner diameter ~2 mm, height 2-4 mm, when DI is made of a ceramic material based on barium titanate ($BaTi_4O_9$ + 8.5% ZnO) with ε~36. This material was chosen thanks to their high purity (no background EPR signals), high quality factor ($Q_f \approx 70000$ at 10 GHz) and low thermal coefficient of the dielectric constant ($T_\varepsilon \cong 0$).

An experimental verification of amplification of the EPR signal with corresponding dielectric insert was performed using $MnCl_2$ powder sample. The application of this DI for the X-band CW Varian E12 EPR spectrometer was found to increase the intensity of the EPR signal by 6.5 times.

[1] Golovina I. S., Geifman I. N., Rodionov Ye. V. Dielectric resonators for EPR spectroscopy. - Kiev. Institute of Semiconductor Physics of NAS of Ukraine. - 2015.- 158 p.

EFFECT OF ORTHO- AND PARA-SUBSTITUTIONS IN AZO-NAPHTHOL DYES ON THE DIFFRACTION EFFICIENCY OF HOLOGRAPHIC MEDIA

Dmitry Vyshnevsky[a], Valeriia Ovdenko[a], Alexander Ishchenko[b], Irina Kurdyukova[b], Nikolay Davidenko[a], Elena Mokrinska[a], Valeriy Pavlov[a]
[a] *Taras Shevchenko National University of Kyiv, 60 Volodymyrska St., Kyiv 01033, Ukraine.*
e-mail: vyshnevsky@protonmail.com
[b] *Institute of Organic Chemistry, NAS of Ukraine, Murmans’ka Str., 5, 02660, Kyiv, Ukraine.*

Films of polymer composites containing azo dyes in main/side polymer chain or as dopants can be used in development of electro-optical modulators of light and recording information media (RIM) for polarization holography. In azo-containing materials photoinduced optical anisotropy appears under linearly polarized light irradiation. This effect is caused by the processes of trans-cis isomerization of azobenzene groups. In this case, substitution effect is very important for future modeling of efficient RIM.

In this work we have studied the dynamic holographic capabilities of poly(styrene-co-nonylmethacrylate) (PSN) thin films doped with two isomeric azo dyes: 4-((4-ethoxyphenyl)diazenyl)naphthalen-1-ol (A1) and 1-((4-ethoxyphenyl)diazenyl)naphthalen-1-ol (A2). Both isomers were investigated and compared using a polymer matrix with a low softening point (~ 38°C). It was found, that the values of diffraction efficiency in the case of the ortho-isomer are approximately 2.5 times higher than the values of diffraction efficiency for the para-isomer in both cases of data beam polarization, perpendicular and parallel to the reference beam. This may indicate that the changes in the dipole moment in case of para-substituted azo compound are larger and, as a result, cause formation of a deeper surface relief.

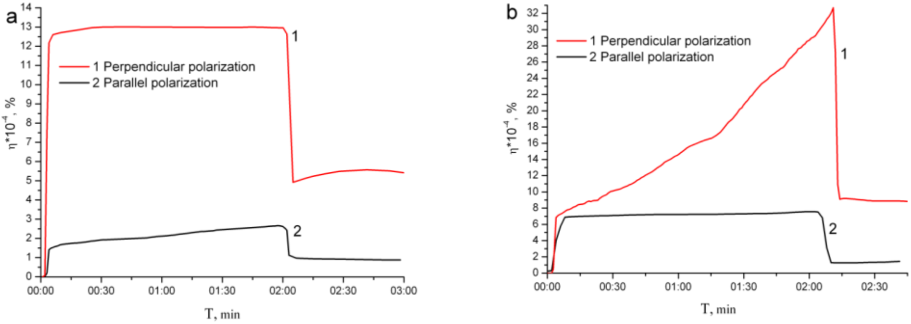


Figure 1. The diffraction efficiency changes in A1/PSNM (a) and A2/PSNM (b) films for parallel and perpendicular data beam polarization

INNOVATIVE SENSOR SOLUTIONS BASED ON YANSON POINT CONTACTS

G.V. Kamarchuk[a], A.P. Pospelov[b], A.V. Yeremenko[a], L.V. Kamarchuk[c,d], A.V. Kravchenko[d]
[a] *B. Verkin Institute for Low Temperature Physics & Engineering, 47 Nauky Ave., Kharkiv, 61103, Ukraine*
[b]*National Technical University "Kharkiv Polytechnic Institute", 2 Kyrpychov Str., Kharkiv, 61002, Ukraine*
[c]*SI "Institute for Children and Adolescents Health Care" of NAMS of Ukraine,52-A Yuvileinyi Ave., Kharkiv, 61153, Ukraine*
[d]*V.Karazin Kharkiv National University, 4 Svobody Sq., Kharkiv, 61077, Ukraine*
e-mail: kamarchuk@ilt.kharkov.ua

The field of sensors has undergone rapid progress and is currently in focus of world-wide research combining physics, chemistry, biology and materials science. One of the perspective trends in this activity is development of sensors based on various nanoobjects. This has already resulted in a large variety of sensor devices and applications for them. Essential improvement in existing nanosensor techniques can be reached through discovery of new sensor approaches based on advanced fundamental benchmarks that have not been applied up to now. In this view, point contact sensors demonstrate high prospects and are able to provide breakthrough in sensor performance to a new technological level.

Point-contact sensors are an emerging trend in modern nanosensor techniques. They are based on advanced investigations of an essentially fundamental concept, namely, that of Yanson point-contact spectroscopy, and on strong "know-how" of technology of Yanson point contacts [1]. Among distinctive features of the point-contact sensor approach are newly proposed original topics in sensorics which have no analogues in the world and will ensure development of innovative technologies operating at the detection limit of sensor devices. In this view, we would like to note the point-contact method for spectral analysis of complex gas mixtures which does not require detection of separate components of the gas mixture under study and the method for quantum detection of liquid and gaseous media resulting from the discovery of a new quantum selective detection mechanism in Yanson dendrite point contacts [2, 3]. Basic properties of Yanson point contacts allow them to work as a spectroscopic and quantum sensory tool which opens up new opportunities for various applications.

This work was partly supported by the NATO SPS Programme (Ref: SPS 985481).

[1] G.V. Kamarchuk, A.P. Pospelov, L.V. Kamarchuk, and I.G. Kushch, Point-Contact Sensors and Their Medical Applications for Breath Analysis: A Review, in: *Nanobiophysics: Fundamentals and Applications*, edited by V.A. Karachevtsev, (Pan Stanford Publishing, Singapore, **2015**), 327-379.

[2] I. Kushch, N. Korenev, L. Kamarchuk, et al., *J. Breath Res*., **2015**, 9(4), 047111.

[3] G.V. Kamarchuk, A.P. Pospelov, A.V. Savytskyi, A.O. Herus, Yu.S. Doronin, V.L. Vakula, E. Faulques, *SN Applied Sciences*, **2019**, 1:244.

CHEMICAL TREATMENT OF Cd (Mn)Te SURFACE

L.M. Kanak, V.G. Ivanitska, P.M. Fochuk
Chernivtsi National University, Kotsyubynskogo st. 2, Chernivtsi, 58012, Ukraine
e-mail: tkachuklilya98@gmail.com

CdTe and his solid solutions - Cd(Mn)Te and Cd(Zn)Te - have proven to be effective materials for room temperature X-ray and gamma ray detection with a number of applications in nuclear safety, medical imaging, transportation safety etc. The possibility of practical application is often limited by surface conditions. In our previous studies it was shown that iodine-based solutions can be used for successful A^2B^6 semiconductor surface treatment [1].

We report here on development of the iodine based etching system KIO_3-KI-tartaric acid ($C_4H_6O_6$), which was chosen as a candidate for final polishing of Cd(Mn)Te surface. Iodine is created by the interaction between KIO_3 and KI source components. Addition of tartaric acid in etchant solution reduces the etching velocity due to enhancement of the etchant viscosity. In addition, citric acid promotes more effective removing of reaction products from Cd(Mn)Te surface.

Samples under investigation were cut from $Cd_{0,95}Mn_{0,05}Te$ non-oriented single-crystal. The 5 % KIO_3, 55 % KI and 25 % $C_4H_6O_6$ aqueous solutions were used as mother solution for etchant preparation. Semiconductor dissolution was carried out in reproducible hydrodynamic conditions using chemical dynamical polishing equipment. Study of etching rate dependences on etchants chemical compositions was carried out at room temperature at disk rotation speed of 84 rpm. The etching rate was evaluated by reducing the thickness of the sample per unit time. Mathematical simulation of experimental data, using the simplex-method, was applied and etchant composition optimization for polishing treatment of Cd(Mn)Te surface was carried out.

The $Cd_{0,95}Mn_{0,05}Te$ dissolution rate in KIO_3–KI–$C_4H_6O_6$ etching solutions was found to vary from 0,5 to 8 μm/min. The maximum of dissolution rate was observed in solutions, enriched by potassium iodate and potassium iodide simultaneously. The etched semiconductor surfaces were smooth, clean and visible films free. The dependence of the etching rate versus time of solution storage was studied. It was shown that KIO_3–KI–$C_4H_6O_6$ etching system can be characterized as age resistance. The polishing properties of etchants did not disappear over the whole period of solution storage. One can conclude that KIO_3–KI–$C_4H_6O_6$ etchant compositions can be used for polishing of Cd(Mn)Te surface and controlled removal of semiconductor material.

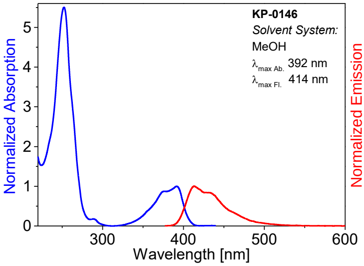
[1] V.G. Ivanits'ka, P. Moravec, V.M. Tomashik, K. Masek, Z.F. Tomashik, J. Franc, R. Grill, P. Hoschl. A slightly oxidizing etchant for polishing of CdTe and CdZnTe surfaces / J. Electron. Mater. – **2013**. – Vol. 42, № 11. – P. 3059 – 3065.

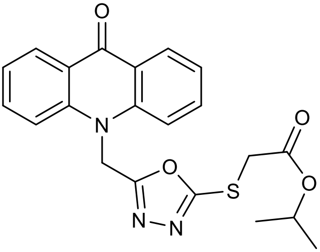
OPTICAL PROPERTIES OF THE NEW 10-((1,3,4-OXADIAZOLES-2-YL)METHYL)ACRIDINE-9(10H)-ONES

Yu. V. Karpenko, A. I. Panasenko
Zaporizhzhia State Medical University, *Maiakovskyi avenue 26, Zaporizhzhia 69035, Ukraine*
e-mail: karpenko.y.v@gmail.com

The emergence of the latest technologies and fields of practical application requires the creation of dyes and phosphors with improved characteristics and specific properties. Acridine-9(10H)-one is very photostable, has high absorption at 405 nm and emits at 550 nm, luminescence duration is 14.9 ns, quantum yield equals 0.8 in water. In addition, many derivatives containing acridine-9(10H)-one exhibit blue-violet fluorescence (λ_{abs} = 384 nm, λf_l = 441 nm), which is advantageous for visualizing their activity in cell cultures or tissue samples.

Spectral studies of the dilute solution of the synthesized organic compound were carried out in a spectrally pure solvent, methanol.





Agent	$\lambda_{abs.}$, nm	$\lambda_{fl.}$, nm	Stokes shift, nm	φ, %
Methanol	392	414	22	78

Increasing of the carbon chain attached to the Sulfur atom decreases the quantum yield of fluorescence, which is associated with a decrease in the manifestation of the 1,3,4-oxadiazole acceptor effect. It was noted that such an influence of alkyl groups may be associated with their participation in the stabilization of the resulting photoexiton disruption. Based on the above, we have proposed a compound as a new fluorescent dye, probe and tap, suitable for applications based on the analysis and quantification of proteins and nucleic acids of DNA and RNA, in immunology - for the observation of the interaction of antigens with antibodies based on the interaction of complementary pairs of oligonucleotides, for obtaining biological images by fluorescence microscopy and for solving other medical and biological problems.

FEATURES OF TRANSFORMATIONS IN SYSTEMS OF NITRATE PRECURSORS OF LANTHANOIDS AND ALKALINE METALS IN THE FORMATION OF PHOTOCATALYTIC ACTIVE NANO-LAYERED PEROVSKITE-LIKE PHASES

O. Dryuchko, D. Storozhenko, N. Bunyakina, I. Ivanytska, I. Gornitsky,
V. Khaniukov, K. Kytaihora
Poltava National Technical Yuri Kondratyuk University, Pervomaysky prospect, 24, Poltava, 36011, Ukraine, e-mail: dog.chemistry@gmail.com

The report goes on to discuss and analyze the results of a study of the features of the common behavior of structural components in the systems of precursors of lanthanide nitrates and alkali metals at preparatory stages during the formation of REE-containing oxides with perovskite structure, pomegranate using "soft chemistry" and thermal activation.

One of the most promising classes of rare earth oxide and titanium complex oxide materials is nanostructured layered perovskite-like compounds (the Raddlesden-Popper, Dion-Jacobson phases) and solid solutions based on them.

New information on the reactivity and transformation of layered perovskite-like oxides, stabilization of photocatalytic and sensor-active crystalline modification of TiO2 - anatase initiated the continuation of our research on this topic. And today the ways of managing the technical parameters of the target products through the choice of composition, synthesis conditions and processing method are being clarified.

Now, thanks to technological techniques of "soft chemistry" reactions, it has become possible to create substances with various structural features, to obtain metastable compounds by a sequence of low-temperature topochemical syntheses. Of particular interest in this regard are hybrid synthesis methods that combine the advantages of each of the methods used (elements of pyrolysis and hydrolysis synthesis methods, liver method, combustion of liquid nitrate precursors, sol-gel method) and use liquid nitrate precursors of elements of different electronic structures.

Ion exchange, intercalation and deintercalation, substitution and condensation processes, splitting processes, and mutual transformations of one structure to another are used to form the target phases (for example, the transition from the Raddlesden-Popper phase to the Dion-Jacobson phase; transition within one type of phases with increasing reducing the number of layers).

The empirical data obtained by the authors [1] on the conditions of formation and existence, on the peculiarities and regularities of the atomic-crystalline structure, properties, character and stability of thermal transformations of alkaline coordination nitrates of lanthanides play an important role in optimizing the development of technologies for the production of new multifunctional REE-containing materials. They are an important stage in the development of an experimental and theoretical scientific database on layered compounds and the processes involved; their unique properties, which are determined by the two-dimensional nature of the construction of the interlayer space, the distortion of the structure of titanium-oxygen octahedra of the perovskite layer and the high mobility of alkali metal cations.

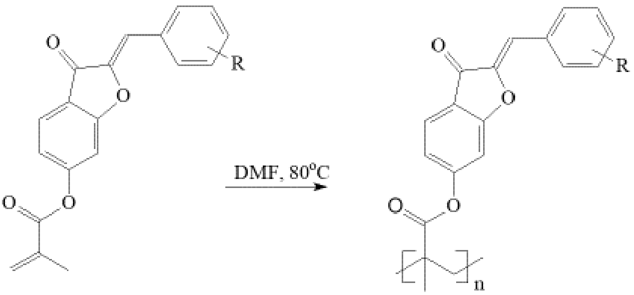
[1]References: O. Dryuchko, D. Storozhenko, A. Vigdorchik, N. Bunyakina, I. Ivanytska, K.Kytaihora, V. Khaniukov. *Molecular Crystals and Liquid Crystals*. (2018), 672(1), 199-214.

INFLUENCE OF SUBSTITUENT ON POLYMERIZATION ABILITY OF METHACRYLIC MONOMERS BASED ON AURONE FRAGMENT

O. Kharchenko, D. Shyrchenko, V. Smokal, O. Krupka
Department of Macromolecular Chemistry, Taras Shevchenko National University of Kyiv, 60 Volodymyrska St., Kyiv, Ukraine,01033
e-mail: oksana_kharchenko@ukr.net

The development of information technologies requires more concepts for creation new multifunctional materials and study its function-structure relationships. The most important among them are polymer photochromic materials, which can be observed by few ways. The first method is mechanical mixing of polymer matrix and chromophore. The second method involves the covalent introducing of chromophore molecule in the main chain of polymer or as side-on attached [1]. Materials synthesized by second way have some advantages: solubility, film coating, time stability, adhesion, conductivity, etc., and can find application in optics, photovoltaics, photonics, medicine and many others.

In this work we present synthesis and investigation of polymerization activity of new monomers based on 6-hydroxyaurone fragment. The common structures of synthesized methacrylic monomers and polymers is representing below:



M1-M3 P1-P3

, where R = -Cl in ortho- (**M1**, **P1**), meta- (**M2**, **P2**) and para-position (**M3**, **P3**)

Novel monomers were synthesized by using methacryloyl chloride for acylation 6-hydroxyaurone derivatives at basic conditions and low temperatures.

The polymerization ability of the new monomers was investigated kinetically for radical thermal initiated polymerization by dylatometric method. The polymerization was carried out for 10% solution of monomer in DMF with 1% of AIBN as initiator at 80°C. The structure of synthesized compounds was determined by ^{1}H NMR-spectroscopy.

[1] M. Ya. Goikhman, *Polymer Science,* Ser. B, **2014**, Vol. 56, No. 3, pp. 352–359

PECULIARITIES OF ELECTRON-PHONON INTERACTION IN THE INDIUM SELENIDES:*Ab INITIO* INVESTIGATION

L.Yu.Kharkhalis, K.E.Glukhov, T.Ya.Babuka, M.V.Liakh
Institute of Physics and Chemistry of Solid State, Uzhhorod National University,
54 Voloshin Str., 88000 Uzhhorod, Ukraine
e-mail: lkharkhalis@gmail.com

Electron-phonon interaction in the indium selenide crystals is the subject of an intense theoretical and experimental study. It is known that the interaction of electrons with phonons can affect the electrical conductivity and thermal conductivity and, accordingly, the thermoelectric efficiency of materials. As we have previously shown, the interaction of electrons with acoustic longitudinal oscillations in In_4Se_3 homeopolar crystals can lead to the formation of self-consistent localized states of the large radius, called condensons (polaron analog) [1]. Our concept of condenson states for In_4Se_3 crystal is used to explain its high thermoelectric figure of merit [2,3]. Recently, in [4] it was shown that electron-phonon coupling in the single-layer InSe is anomalously strong owing to the peculiar character of hole states and their interaction with phonons. As it is followed from our investigations the electron spectra of the In_4Se crystal is also characterized by the dispersive dependence by the "Mexican hat" type [1] similar to one of InSe monolayer [5]. Therefore, for both bulk In_4Se_3 and β-InSe crystals, it is of considerable interest to study the electron-phonon coupling which can play an important role in the transport phenomena and optical properties of considered materials.

Utilizing the program packet ABINIT with the application of the updated methodology of the density functional perturbation theory (DFPT), we investigated the interaction between the electron and phonon subsystems for the In_4Se_3 and β-InSe crystals. The phonon spectra, the density of phonon states, the Eliasberg spectral function $\alpha^2F(\omega)$, electron-phonon coupling strength λ and the phonon linewidths $\Gamma_{el\text{-}ph}$ have been calculated. Analyzing the frequency bandwidths and the distribution and intensity of spectral function $\alpha^2F(\omega)$ we obtained the increase in the intensity of electron-phonon interaction in In_4Se_3 crystal in comparison with the bulk β-InSe. This fact stimulates the search for new effects of optical and transport properties, similar to those found in InSe monolayer [4].

---

[1] D.M.Bercha, L.Yu.Kharkhalis, A.I.Bercha, M.Sznajder, *Phys. Stat. Sol (b)*, **1997**, 203, 427.

[2] Y.S. Lim, M. Jeong, W.-S.Seo, J.-H.Lee, C.H.Park, M. Sznajder, L.Yu.Kharkhalis, D.M. Bercha, J.Jang, *J.Phys.D.: Appl.Phys.*, **2013**, 46, 275304.

[3] M.Jeong, Y.S.Lim, W.-S.Seo, J.-H.Lee, Ch.-H. Park, M.Sznajder, L.Yu.Kharkhalis, D.M.Bercha, J.Yang, *Journ. of Materials Chemistry A.*, **2013**, 1, 15342.

[4] A.V.Lugovskoi, M.I.Katsnelson, A.N.Rudenko, *Physical Review Letters*, **2019**, 123, 176401.

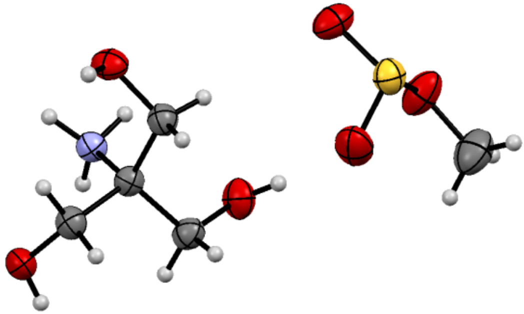
[5] M. J. Hamer, J. Zultak, A. V. Tyurnina, V.Zolyomi, *ACS Nano*, **2019**, 13, 2136.

THE PRODUCTS OF SO_2 INTERACTION WITH ALCOHOL SOLUTIONS OF TRIS(HYDROXYMETHYL)AMINOMETHANE

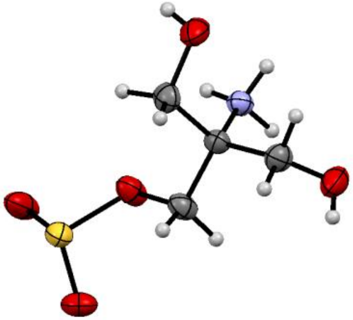
Khoma R.E.[a,b], Dlubovskiy R.M. [a], Baumer V.N.[c], Ennan A.A.-A.[a],
Ishkov Yu.V.[b], Vodzinskiy S.V.[a,b], Gelmboldt V.O.[d]
[a]*Physico-Chemical Institute of Environment and Human’ Protection,*
Preobrazhenskaya St., 3, Odessa, 65082, Ukraine
[b]*Mechnikov Odessa National University, Dvoryankaya St., 2, Odessa, 65082, Ukraine*
[c]*Institute of Single Crystals, National Academy of Sciences of Ukraine,*
Nauky ave., 60, Kharkov, 61072, Ukraine
[d]*Odessa National Medical University,Valikhovskiy lane, 2, Odessa, 65082, Ukraine*
e-mail: rek@onu.edu.ua

The new methods of preparation of sulphurous esters via interaction in the SO_2 – $(HOCH_2)_3CNH_2$ – AlkOH systems (Alk is methyl, ethyl, *n*-propyl, and *i*-propyl) have been developed. The compounds were characterized by elemental analysis, X-ray diffraction, Raman, IR, ^1H, ^{13}C NMR spectroscopy and mass spectrometry.

The crystal structures of new esters: tris(hydroxymethyl)methylammonium methylsulphite (**I**), [2-amino-3-hydroxy-2-(hydroxymethyl)propyl]hydrosulphite (**II**) with the compositions $[(HOCH_2)_3CNH_3^+]\cdot[H_3COSOO^-]$ and $^+NH_3C(CH_2OH)_2CH_2OSO_2^-$ have been determined by X-ray diffraction. The structures of **I** and **II** are stabilized by numerous H-bonds NH···O, OH···O.



I



II

Ammonium methylsulphite: **I** monoclinic space group *P2₁/c* with the following cell parameters: $a = 8.2170(5)$, $b = 6.2840(5)$, $c = 18.4669(9)$ Å, $\alpha = 90.00$, $\beta = 95.299(5)$, $\gamma = 90.00°$, $V= 949.475$ Å^3, $Z = 4$. Ammonium hydrosulphite **II** of zwitterionic structure crystallizes in the monoclinic space group $P2_1/c$ with the following cell parameters: $a = 6.9493(6)$ Å, $b = 9.8955(9)$ Å, $c =11.1160(10)$ Å, $\beta = 93.604(8)°$, $V= 762.9$ Å^3, $Z = 4$.

New examples of stabilization diethylsulphite in the form of molecular complex in the SO_2 – $(HOCH_2)_3CNH_2$ – C_2H_5OH system have been demonstrated. The formation molecular complex is the result of interaction following the scheme:

$$SO_2 + (HOCH_2)_3CNH_2 + 2C_2H_5OH \rightarrow (C_2H_5O)_2SO\cdot NH_2C(CH_2OH)_3.$$

The spectral characteristics of the obtained esters are discussed.

SYNTHESIS, CRYSTAL, AND MOLECULAR STRUCTURES OF 3d-METAL 5-SULFOSALICYLATE-BENZOHYDRAZIDE COMPLEXES

Koksharova T.V.[a], Savchenko O.[b], Mandzii T.V.[a]
[a] *I.I. Mechnikov Odessa National University, Dvoryanskaya St., 2, Odessa, 65082, Ukraine*
[b]*Ecotech-complex,University of Maria Curie-Skłodowska, Lublin, Poland*
e-mail: tanya.koksharova@gmail.com

The complexes of Co(II), Ni(II), Cu(II), and Zn(II) 5-sulfosalicylates with benzohydrazide have been synthesized and studied by IR spectroscopy, diffuse reflection spectroscopy, and X ray diffraction.

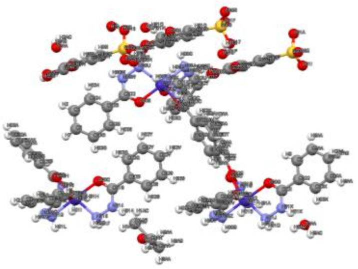


Fig.1. Structure of the cobalt complex

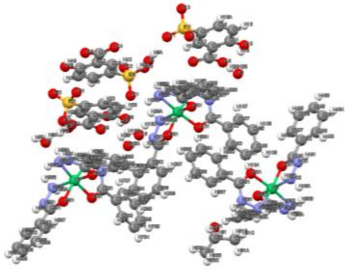


Fig.2. Structure of the nickel complex

It was determined that metal atom is in an octahedral environment, in all compounds. In the case of cobalt and nickel, the crystals contain complex cations $[M(Bhz)_3]^{2+}$, in the outer sphere are anions of doubly deprotonated sulfosalicylic acid H_3Ssal molecules.

In the case of copper and zinc, isostructural complexes are obtained in which the crystals are made of neutral molecules $[M(Bhz)_2(H_2SSal)_2]$, where the five-membered hydrazide ligand metallocycles lie in the same plane and oxygen atoms of two sulfogroups $H_2Ssal^-$are in the axial position, thus adding a coordination polyhedron to the octahedron. The copper complex is stabilized by the intrasphere sulfosalicylate anion.

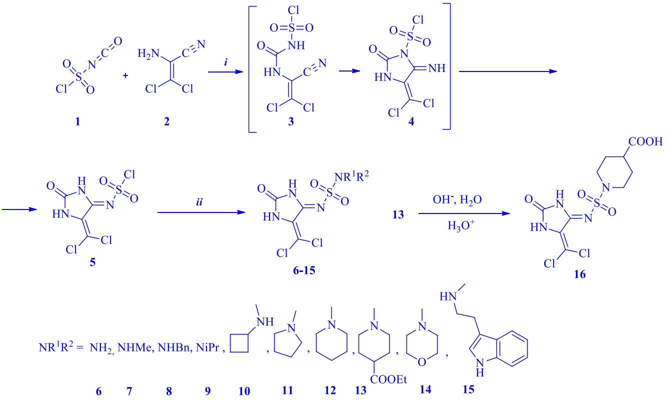
Fig.3. Structures of copper and zinc complexes

NEW 2-OXOIMIDAZOLIDINE DERIVATIVES: DESIGN, SYNTHESIS AND EVALUATION OF ANTI-BK VIRUS ACTIVITIES IN VITRO

Kornii Yurii, Oleh Shablykin, Volodymyr Brovarets
V. P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry, NAS of Ukraine, 1, Murmanska Str., Kyiv 02094, Ukraine
e-mail: s8092011@ukr.net

Imidazolidine nuclei have beenattracting considerable attention in various fields owing to their unique structures and characteristics. Recently, the chemistry of 2-oxo-imidazolidine derivatives has been receiving attention due to their various efficient biological importance. Imidazolidinones possess potent activities against several viruses such as dengue virus, enterovirus, hepatitis C virus (HCV), and human immunodeficiency virus (HIV). Therefore, 2-oxoimidozalidine derivatives have quite attractive antiviral properties. Human polyomavirus 1 (BKPyV) is DNA circular double-stranded virus. These viruses are often latent in the host organism, but form tumors in the event of host immune deficiency. There is anurgent need for development of a safe and efficacious antiviral agent against BK virus, as well as a prophylactic vaccine. Therefore, further research exploring new effective compounds in the treatment of human polyomavirus associated diseases is required. In the present study, the antiviral potential of new 2-oxoimidazolidine derivatives against BKPyV (strain Gardner) were investigated on HFF cell lines.

The synthetic procedure of compounds



(i) Et2O abs., 30-35°C, 14h; (ii) R1R2NH (6 eq), THF, 20-25°C, 6h, then HCl aq.

In general, all the synthesized novel 2-oxoimidazolidine derivatives exerted some degree of antiviral activity in vitro against the BKPyV. A series of 2-oxoimidazolidines derivatives was designed, synthesized and evaluated for their anti-BKPyV activities. The biological screening results indicated that some compounds were found to have moderate activity against BKPyV. In some parameters, these compounds are not inferior to Cidofovir. Hence, these compounds may be taken as lead compound for further development of novel anti-BKPyV agents.

POLYMER COATED MAGNETIC NANOPARTICLES

Korobeinyk A.V., Tertykh V.A.
O.O. Chuiko Institute of Surface Chemistry of National Academy of Science of Ukraine
17, Gen. Naumov Str., 03164 Kyiv, Ukraine
e-mail: alina.v.korobeinyk@gmail.com

Synthetic magnetite nanoparticles (MNPs) have been in focus of many researches due to their unique properties associated with the size/magnetization ratio. Such nanoparticles show the advantages in drug delivery and cancer thermal therapy [1].

MNPs were prepared by precipitation of ferrous ions in the presence of carboxymethyl cellulose (CMC) at high pH in order to achieve high dispersibility and a protective polymer coating. X-ray diffraction study (Fig. 1) indicates the presence of only magnetite phase (JCPDS card #3-0863) with the average particle sizes calculated to be 6.3 nm (from highest peak intensity plane (311)), using the Sherrer`s equation.

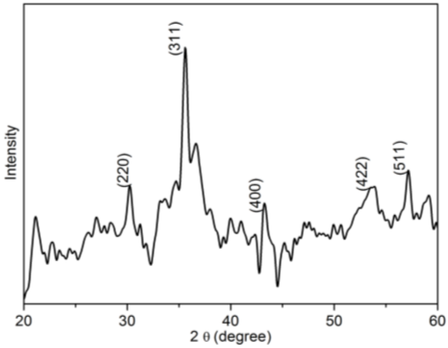


Fig. 1. XRD pattern of MNPs.

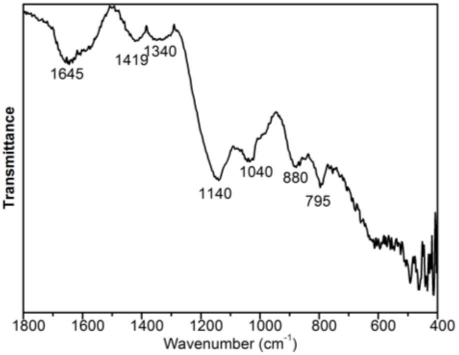


Fig 2. FTIR spectrum of MNPs.

The infrared spectrum (Fig. 2) shows absorption at 434. 465, 494, 795 and 880 cm^{-1} corresponding to Fe-O vibrations of Fe_3O_4 and bands at 1040, 1140, 1340, 1419 and 1645 cm^{-1} associated to the CMC presence. The polymer bonds are shifted slightly compared with neat CMC due to the MNPs presence.

The main conclusion is that synthesized MNPs have potential in hyperthermia treatments. Future research will be focused on the using of different coatings for MNPs and study of their colloidal and magnetic properties.

[1] Ito, A., et al., *Journal of Bioscience and Bioengineering*., **2005**, 100(1), 1-11.

EVALUATION OF THE POLYURETHANE BASED LASER ELEMENTS PHOTOSTABILITY AND BEAM STRENGTH

L. Kosyanchuk[a], N. Kozak[a], N. Babkina[a], T. Bezrodna[b],V. Bezrodnyi[b], O. Antonenko[a]

[a] *Institute of Macromolecular Chemistry NAS of Ukraine, 48 Kharkiv chaussee., Kyiv 02160, Ukraine*
[b]*Institute of Physics NAS of Ukraine, 46 Nauki av., 03680 Kyiv, Ukraine*
kozaksmalt@ukr.net

The use of polyurethane-based polymer matrices allows to provide stable operation of the dye lasers [1,2]. Among the main requirements, which should be met by the polymer matrices in dye laser solid-state elements, their photostability and beam strength are crucial factors. Effects of irradiation on structure and photostability and beam strength of the polyurethanes with a use of different diisocyanate and glycol components have been investigated. Here photostability is understood as polymer resistance to photooxidation and photochemical destruction, and beam strength means ability of the material to withstand irreversible changes of its optical parameters and retain integrity under strong optical irradiation (in particular, by a laser), including stability to local overheating. This work presents a comparative analysis of photooxidation destruction characteristics for different PU polymers, and their beam strength parameters, obtained by various methods (IR-spectroscopy, dynamic mechanical analysis, paramagnetic probe and laser experiments).

Photooxydation processes are shown to change elasticity of the materials, glass transition temperature and average molecular mass for the chain segments between polymer cross-linked points, and also induce accumulation of hydroxyls in the system due to the formation of alcohol and hydroperoxide groups. Beam strength of the polyurethanes is found out to be dependent on the polymer chemical structure, in particular, on a length of the aliphatic block and density of the cross-linking network. Good agreement between the results obtained by the dynamic mechanical analysis, IR-spectroscopy, EPR methods and the data for the single-pulse laser destruction thresholds allows to predict photooxidation susceptibility for the further developed polyurethane materials.

[1] L.Kosyanchuk, T.Bezrodna, M.Stratilat, T.Todosiichuk, J. Pol. Res., **2014,** 21, 564–571

[2] L Kosyanchuk, N. Kozak, N. Babkina, V. Bezrodnyy, M. Stratilat, Fr.-Ukr. Chem. J.,**2016**, 4, 40–46.

PREPARATION OF POLYLACTIC ACID/SILICA COMPOSITES USING THE *IN SITU* RING-OPENING POLYMERIZATION OF LACTIDE

Kozakevych R.B., Polyshchuk L.M., Tertykh V.A.
Chuiko Institute of Surface Chemistry, NAS of Ukraine, 17 General Naumov Str., 03164 Kyiv, Ukraine *e-mail: kozakevych@gmail.com*

Polylactide (PLA) is a biodegradable, aliphatic polyester, which decomposes completely to harmless and non-toxic decomposition products under natural conditions [1]. This property of polylactide allows it to be a more attractive material to replace traditional petroleum-based polymers. Due to its biocompatibility, complete biodegradability and non-toxic nature of degradation products, PLA based polymeric materials has become attractive material for preparation of various polymeric devices used for different medical applications, tissue engineering, adsorbent material and drug delivery systems [2].

A novel method of grafting ring-opening polymerization of *L*-lactide onto the surface of pyrogenic silica (A-300) and modified with 3-aminopropyltriethoxysilane (APTES) silica (A-NH_2) was carried out. The *L*-lactide oligomer was grafted onto the surface of silica nanoparticles through condensation reaction of *L*-lactic acid in the presence of stannous octoate catalyst and without it. The surface-grafting reaction was confirmed by FTIR, TGA data.

The IR spectra of fumed silica (A-300), modified silica (A-NH_2) nanoparticles before and after grafting of lactide with and without catalyst are shown in Fig 1 and 2.

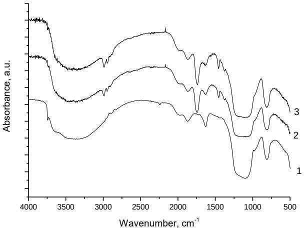


Fig. 1. FTIR-spectra of A-300 (*1*), composite A-300/PLA (*2*), composite A-300/PLA with $[Sn(Oct)_2]$ (*3*)

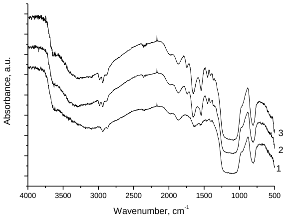


Fig. 2. FTIR-spectra of A-NH_2 (*1*), composite A-NH_2/PLA (*2*), composite A-NH_2/PLA with $[Sn(Oct)_2]$ (*3*)

The fumed silica A-300 is characterized by the absorption bands at 1090 and 800 cm^{-1} which can be ascribed to stretching and bending vibrations of Si-O-Si bonds. After surface PLA grafting, a new absorption band appears at 1740 cm^{-1}. The new peak is attributed to the carbonyl group (C=O) of PLA, confirming the grafting of *L*-lactic acid oligomer onto the surface of SiO_2 nanoparticles. After modification of silica nanoparticles with APTES (Fig. 2), the new peaks can be assigned as follows: the new band (1564 cm^{-1}) is due to N–H bending vibration of amino groups, the band at 3501 cm^{-1} can be assigned to N–H stretching vibration. After surface PLA grafting the infrared absorption spectra exhibit appearance of characteristic band in the region of 1640 cm^{-1} assigned to azomethine bonds in the surface compounds formed between aminopropyl groups and polylactide.

[1] Garlotta D., A literature review of poly (lactic acid), *J. Polym. Environ.*, **2002** , 9(2), 63 – 84.

[2] Sodergard A., Stolt M., Properties of lactic acid-based polymers and their correlation with composition, *Prog. Polym. Sci.*, **2002** , 27**,** 1123 – 1163.

ACTIVATED CARBON (AC) – TITANIUM DIOXIDE (TiO_2) COMPOSITES: EFFECT OF AC PROPERTIES ON PHOTOCATALYTIC EFFICIENCY

Anzhela Kukh, Irina Ivanenko, Igor Astrelin
National technical university of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute",
37, Prosp. Peremohy, Kyiv, Ukraine, 03056
e-mail: angela.kukh@gmail.com

Electron-hole recombination is one of the drawbacks of photocatalytic processes. It prevents the formation of hydroxyl radicals. The surface of AC may contain a certain amount of metallic compounds, which may act as dopants of the catalytic matrix that promote hole stability. It was investigated, that dopant metallic ions act as electron scavenges [1]. However, doping that exceeds 10% tends to decrease photocatalytic efficiency.

The low-temperature sol-gel method was developed for the synthesis of pure titanium dioxide, as well as samples of "activated carbon-TiO_2" composites [2]. Due to the fact, that synthesis of samples employs doping with KF, the selection of inert support should be careful, so its chemical properties do not interfere with photocatalytic process efficiency. The ash content (non-combustible fraction) of AC was used as one of the reasons for the selection of AC for composites. ACs presented in table 1 were considered for the synthesis of samples.

Table 1 — Activated carbons considered for the synthesis of composites

No.	Tradename of AC	Ash content, %
1	BAU	6
2	Filtrasorb 400 (F400)	4
3	Filtrasorb 300 (F300)	6
4	Norit SAE Super	4

ACs BAU and Filtrasorb 300 were excluded based on a high percentage of ash content. Composites synthesized with activated carbons F400 and Norit SAE Super were further investigated in comparative photocatalytic studies using isopropyl (IP) alcohol as a model pollutant (table 2).

Table 2 — Comparative photocatalytic studies using isopropyl (IP) alcohol

Tradename of AC	C_0(IP), %	C_{res}(IP), %	Removal efficiency, %
F400	20	16,4	18
Norit SAE Super	20	15	25

Thus, Norit SAE Super was selected as an inert support for the synthesis of composites.

[1] Li X.Z., Li F.B. Study of Au/Au^{3+}-TiO_2 photocatalysts toward visible photooxidation for water and wastewater treatment. *Environmental Science and Technology*. **2001**.35, 2381-2387.
[2] Kukh A.A., Ivanenko I.M., Astrelin I.M. TiO_2 and its composites as efective photocatalyst for glucose degradation processes. *Applied Nanoscience*. **2018**. 9, 677-682.

SYNTHESIS AND CHARACTERIZATION OF CdS NANOPARTICLES GROWN IN THE STAR-LIKE COPOLYMER

Yu. Kuziv, H. Hrytsko, N. Melnik, V. Pavlenko, N. Kutsevol
Faculty of Chemistry, Taras Shevchenko National University of Kyiv, 60 Volodymyrs'ka str., 01601 Kyiv, Ukraine
e-mail: garaguts.yulia.fox@gmail.com

Semiconductor nanoparticles are of great interest due to their unique size-dependent optical and electronic properties, also via application in light-emitting diodes (LEDs), electrochemical cells, lasers, hydrogen production catalysts, and biological tags. Cadmium Sulfide is widely used as a yellow pigment. It is also actively studied as photocatalyst for generating hydrogen from water, material for solar panels and various optoelectronic devices. CdS nanoparticles has been well studied because of distinct established dependence of optical absorption from nanoparticle size, however the synthesis of aggregate stable nanosystems with the narrow dimensional distribution is relevant.

CdS nanoparticles were synthesized in branched star-like copolymers with Dextran core and Polyacrylamide chains starting from different salts, at several temperatures and pH values. The concentration dependence of the formation of cadmium sulfide sols was also investigated. Dynamic light scattering, UV-visible spectroscopy, and Transmission electron microscopy were used to analyze the obtained nanocomposites. It was shown that changes of the anion of the starting salt, as well as temperature and pH values affect the nanoparticle size. The decreasing of the pH and temperature caused the formation of smaller particles and in general more stable CdS sols.

PHYSICO-CHEMICAL BASES FOR THE PREPARATION OF POLYMER-INORGANIC (NANO)COMPOSITES

Galyna Dudok, Iryna Dziaman, Natalia Semenyuk, Khrystyna Kysil, Volodymyr Skorokhoda
Department of Chemical Technology of Plastics Processing,
Lviv Polytechnic National University
Lviv, 12 Bandery str. 79013 Ukraine
e-mail: galyna_lukan@ukr.net

Porous composite materials based on mineral fillers and biocompatible polymer binders are widely used to regenerate damaged bone tissue in biomedical practice. Today, efforts in this field of research are aimed to find the best options for the compound of compositions and structures of composites, as well as practical possibilities for the directed regulation of their properties using various modifying factors and techniques. Among the wide variety of mineral fillers, significant interest is attracted by such fillers as hydroxyapatite (HA), wollastonite, montmorillonite, glass ceramics, etc. The study of the modifying effect of the ultrasonic field on polymers and the initiation of polymerization is of particular interest. Ultrasonic processing is an effective method that allows intensifying technological processes and significantly improving the operational characteristics of composite materials.

We have investigated the regularity of synthesis of polymer composites and nanocomposites based on compositions of 2-hydroxyethylmethacrylate (HEMA) with polyvinylpyrrolidone (PVP) filled with mineral fillers under the action of ultrasound (US), including in the presence of silver nanoparticles. It was revealed that homopolymerization of HEMA without filler does not occur under experimental conditions. The HEMA compositions polymerize at a low rate in the presence of PVP without HA. Mineral fillers form a heterogeneous environment in the compositions. Under the influence of ultrasound, such compositions polymerize very quickly. It is important to note that polymerization is accompanied by simultaneous foaming of the composition. This gives additional technical and economic advantages when developing a technological process for the production of porous composites. The use of ultrasound allows polymerization at a room temperature. The initial polymerization rate in this case is more than 20 times higher than polymerization without ultrasound, even if the latter was carried out at a higher temperature.

The results of this studies on the effect of temperature, ultrasound intensity, nature and amount of filler, as well as monomer concentration on the polymerization rate, made it possible to calculate the kinetic parameters of the polymerization initiated by US. The grafting parameters and the composition of the copolymers are investigated. Depending on the nature of the fillers, under the action of ultrasound, the chemism of the HEMA polymerization reaction in the presence of PVP is proposed. The optimal composition of polymer-inorganic (nano)composites and the conditions for the polymerization of the HEMA-PVP-HA composition under the action of US are selected. The obtained results are used to develop theoretical and applied foundations of the technology for producing osteoplastic composites.

STUDIES OF THE PHYSICAL, OPERATIONAL AND OPTICAL-SPECTRAL CHARACTERISTICS OF THE HIGHLY TRANSPARENT TOLUENESULFONAMIDE AND BENZGUANAMINEFORMALDEHYDE POLYMERS

Vladimir Lebedev[a], Tetiana Tykhomyrova
[a]*National Technical University "Kharkiv Polytechnic Institute", Kyrpychova str., 2, Kharkiv, 61002, Ukraine,*
e-mail: vladimirlebedev1980@ukr.net

To date, there has been much research aimed at finding new transparent polymer bases, to obtain light-sensitive materials based on thermosetting polymers, which are characterized by higher operational characteristics than traditional thermoplastic optically transparent materials. The synthesis and further processing of thermosetting polymers are associated with significant internal stress and chemical shrinkage, which almost always lead to instability of the optical characteristics during operation. At the same time, the filling of the channels and forms in the processing of thermosetting oligomers has considerable specificity and often does not allow obtaining optically transparent products from these materials. No less significant challenges are associated with surface defects of products made of thermosetting oligomers in obtaining transparent parts. Therefore, today obtaining highly transparent polymers of the thermosetting type is quite a challenge. That is why today toluene sulfonamide and benzguanamineformaldehyde polymers – colorless transparent materials, which in their structure have the ability to luminescence are of considerable interest from the point of view of obtaining transparent polymeric materials with luminescent properties.

The researching of the synthesis of toluene sulfonamide and benzguanamineformaldehyde oligomers and polymers with luminescent properties was carried out. The physical-chemical regularities of the process of producing transparent toluene sulfonamide and benzguanamineformaldehyde oligomers and polymers with high spectral-luminescent properties were investigated. It is shown that the modification of oligomers with glycerol with a content of 20 wt % allows obtaining materials with high light transmittance (90–91 %) and low residual stress (10–15 MPa).

The toluene sulfonamide and benzguanamineformaldehyde polymers, which are characterized by low water absorption, high physical–mechanical characteristics when the light transmittance of about 90 % were synthesized. It was found that such an important characteristic of scintillation plastics BAL, in the above-mentioned materials is at the level of PS and PMMA – 40–60 cm to 50–200 cm. It is shown that toluene sulfonamide and benzguanamineformaldehyde polymers are characterized by the extinction coefficient of up to 9000–12000 and the intensity of the luminescence with the relative quantum yield of up to 10 % in the range of 360–365 nm.

MAGNETOTHERMAL PROPERTIES OF LANTHANUM MANGANITE PEROVSKITE NANOPARTICLES

Chunrui Song[a], N.A. Liedienov[a,b], A.V. Pashchenko[a,b,c,d], I.V. Fesych[e], V.G. Pogrebnyak[d], G.G. Levchenko[a,b]
[a] *State Key Laboratory of Superhard Materials, International Center of Future Science, Jilin University, 2699 Qianjin Street, Changchun 130012, China*
[b] *Donetsk Institute for Physics and Engineering named after O.O. Galkin, NASU, Prospekt Nauky 46, Kyiv 03028, Ukraine*
[c] *Institute of Magnetism, NASU and MESU, 36-b Vernadsky Blvd., Kyiv 03142, Ukraine*
[d] *Ivano-Frankivsk National Technical University of Oil and Gas, MESU, 15 Karpatska St., Ivano-Frankivsk 76019, Ukraine*
[e] *Taras Shevchenko National University of Kyiv, 64 Volodymirskaya st., Kyiv 01030, Ukraine*
e-mail: nikita.ledenev.ssp@gmail.com

The unique feature of magnetic nanoparticles is to be heated in an external magnetic field that can be actively used for treating oncological diseases by hyperthermia. For treating many diseases associated with neoplasms, the hyperthermia plays an increasingly important role as a method of local heating. One of the important problems of modern medical hyperthermia is an automatic control of the heating temperature. For obtaining precise control of temperature near 42 °C, the magnetic $La_{0.6}Ag_{0.2}Mn_{1.2}O_3$ nanopowder was synthesized using the nitrate pyrolysis method. The phase composition, structure, morphology, dispersion, magnetic, and magnetothermal properties of the synthesized $La_{0.6}Ag_{0.2}Mn_{1.2}O_3$ nanopowder were studied using XRD, SEM, TEM, and magnetic methods. It has been established that the powder consists of soft magnetic spherical-like nanoparticles with an average size ~ 65 nm. The main magnetic parameters of the nanopowder were determined. Great values of the saturation magnetization up to Curie temperature, sharp magnetic phase transition, and high magnetic homogeneity of the $La_{0.6}Ag_{0.2}Mn_{1.2}O_3$ are due to the influence of superstoichiometric manganese. It was shown that appearance and increase of the specific loss power in the relaxation hysteresis under alternating magnetic field are due to the influence of the Neel relaxation. Intensive heating occurs in the temperature range of 28–42 °C. The obtained values of the specific loss power indicate the possibility of local heating of cell structures for a short time ~ 2 min (Fig. 1). The synthesized magnetic $La_{0.6}Ag_{0.2}Mn_{1.2}O_3$ nanopowder has unique functional properties that can be useful for local hyperthermia.

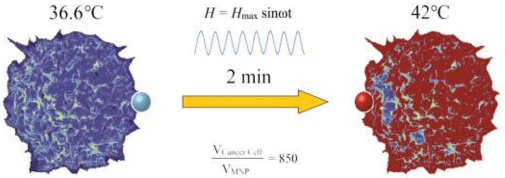


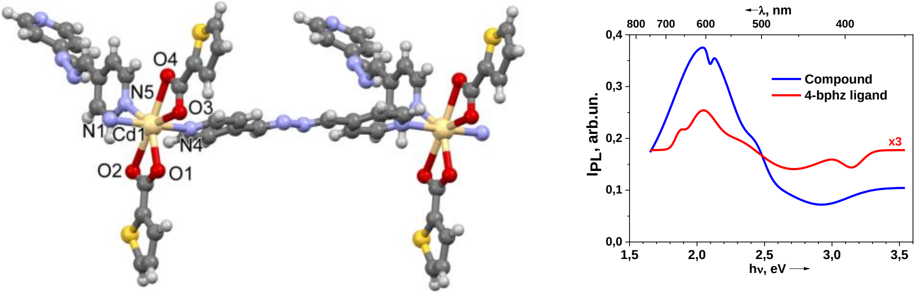
Fig. 1. The simulated process of heating cancer by local hyperthermia method using the $La_{0.6}Ag_{0.2}Mn_{1.2}O_3$ nanoparticle.

LUMINESCENT PROPERTIES OF Cd(II) COORDINATION POLYMER ASSEMBLED FROM 2-THIOPHENECARBOXYLIC ACID AND 1,2-BIS(PYRIDIN-4-YLMETHYLENE)HYDRAZINE LIGANDS

V. N. Lozovan[a,b], O. V. Kulikova[c], V. Ch. Kravtsov[c], E. B. Coropceanu[a,b], M. S. Fonari[c]

[a] *Institute of Chemistry, 3 Academiei str., Chisinau, Republic of Moldova;*
[b] *Tiraspol State University, 5 Iablocikin str., Chisinau, Republic of Moldova;*
[c] *Institute of Applied Physics, 5 Academiei str., Chisinau, Republic of Moldova*
e-mail: lozovanvasile90@gmail.com

The development of lower cost and higher performance phosphor materials for energy efficient lighting and other optoelectronic applications is both necessary and feasible. Luminescent metal–organic frameworks and coordination polymers are a class of materials that hold great promise for this application [1]. Herein we report luminescent properties of one-dimensional coordination polymer, $[Cd_2(4\text{-bphz})_3(2\text{-tpca})_4]_n$ constructed from the semi-rigid Schiff-base N,N'-type ligand, 1,2-bis(pyridin-4-ylmethylene)hydrazine (4-bphz) and 2-thiophenecarboxylic acid (2-tpca) (Figure). Compound crystallizes in the monoclinic $P2_1/n$ sp. gr. The metal coordination node represents mononuclear pentagonal bipyramid with CdN_3O_4 coordination geometry.



(a) (b)

Figure: a) View of Cd coordination core with 4-bphz ligand and partial labeling scheme; b) solid-state emission spectra for 4-bphz ligand and coordination compound

Solid state emission spectra were recorded using a pulse nitrogen laser (λ_{exc} = 337.1 nm) at 300 K. The excitation pulse duration was 15 ns, the repetition frequency was 50 Hz, and the pulse energy was 0.2 mJ. For both the 4-bphz ligand and $[Cd_2(4\text{-bphz})_3(2\text{-tpca})_4]_n$, emission maxima are registered in the region of 2.04 eV. Compound $[Cd_2(4\text{-bphz})_3(2\text{-tpca})_4]_n$ emits 4.5 times stronger than the individual ligand.

[1] W. P. Lustig, J. Li, Coord. Chem. Rev., **2018**, 373, 116–147.

SPR DETECTION OF URANIUM IN AQUEOUS MEDIA USING POLYDOPAMINE FILMS

S. Mamykin[a], I. Gnilitskyi[b,c], M. Dusheyko[d], T. DeVol[e], V. Bliznyuk[e]
[a]V. E. Lashkaryov Institute of Semiconductor Physics, NASU, Kyiv, Ukraine
[b]NoviNano Inc., Lviv, 79021, Ukraine
[c]Department of Photonics, Lviv Polytechnic National University, 79013, Lviv, Ukraine
[d]National Technical University of Ukraine “Kiev Polytechnic Institute”, Kyiv, Ukraine
[e]Environmental Engineering &Earth Sciences, Clemson University, Clemson, SC, USA
e-mail: mamykin@isp.kiev.ua

Polydopamine (PDA) films have a wide application in filtration, energy storage, drug delivery, catalysis and environmental cleaning. PDA can effectively adsorb/absorb heavy metals and radionuclides [1] and, therefore, can be used as the basis for the development of sensors. Among other methods of detection of changes occurring in organic films during their interaction with the environment, surface plasmon resonance (SPR) technique offers high sensitivity, good reproducibility and stability. The most common method of SPR excitation employs either prism or diffraction grating (DG) elements. We have applied the DG-based method [2] with a Semilab SE-2000 spectral multiangle ellipsometer equipped with micro-optics (0.475x0.365 mm light spot size, 75^o angle of light incidence) for detection of the resonance shift associated with uranium soprtion to a PDA film on a substrate.

Typical sensor configuration consisted of a Si substrate with sinusoidal DG on the surface, thin Au film evaporated on the DG and thin uranium sensitive PDA film deposited on top. To form the DG with ~900 nm period we have used surface texturization [3] with femtosecond laser pulses (Yb:KGW laser). An exposure of the system to aqueous solution of uranium salt ($UO_2(NO_3)_2$•$6H_2O$) (1mg/ml) for 43 h led to a shift of the SPR spectral position. A C-method consisting in solution of Maxwell equations in curvilinear coordinates was applied for numerical simulation of the SPR signal. The obtained reflection coefficients R_p for p- (TM mode) and R_s for s- (TE mode) of the polarized light were used for calculation of the ellipsometric angle $\Psi=\mathrm{atan}(R_p/R_s)$.

The SPR shifts from λ=1829 nm for free Au surface to λ=1867 nm after deposition of the PDA film and then to λ=1929 nm after its exposure to the U solution. According to our calculations, the observed shifts of the resonance correspond to a 106 nm average thickness of the deposited PDA film and additional c.a. 50 nm effective thickness of the adsorbed uranium. Considering surface densities of PDA (0.171 g/m^2) and uranyl (UO_2) (0.55 g/m^2) the mass of adsorbed U is about 3 times higher than the mass of the PDA film. This estimation has been confirmed independently by X-ray photoelectron spectroscopy measurements.

[1] V.N. Bliznyuk, K. Kołacińska, A.A. Pud, N.A. Ogurtsov, Y.V. Noskov, B.A. Powell, T.A. DeVol, *RSC Advances*, **2019**, 9, 30052-30063.

[2] A.V. Korovin, N.L. Dmitruk, S.V. Mamykin, V.I. Myn’ko, M.V. Sosnova, *Nanoscale Research Letters*, **2017**, 12, 213.

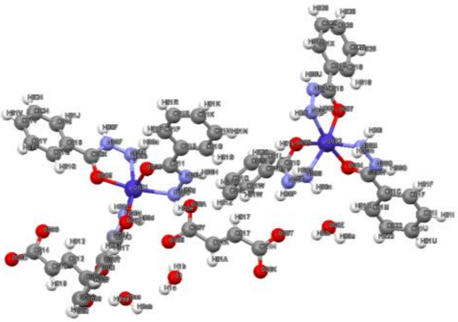
[3] I. Gnilitskyi, V. Gruzdev, N.M. Bulgakova, T. Mocek, L. Orazi, *Applied Physics Letters*,**2016**, 109, 143101.

COMPLEXES OF COBALT AND NICKEL FUMARATES WITH BENZOHYDRAZIDE AND PHENYLACETIC ACID HYDRAZIDE. SYNTHESIS, CRYSTAL, AND MOLECULAR STRUCTURES

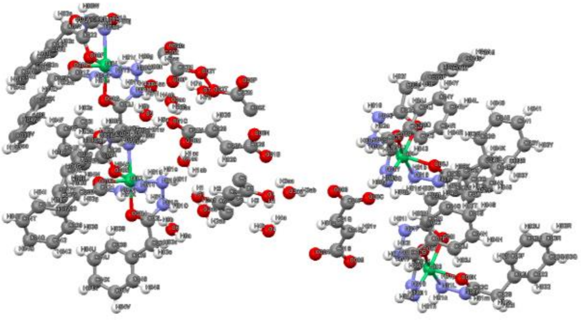
Mandzii T.V.[a], Savchenko O.[b], Koksharova T.V.[a]
[a] *I.I. Mechnikov Odessa National University, Dvoryanskaya St., 2, Odessa, 65082, Ukraine*
[b]*Ecotech-complex,University of Maria Curie-Skłodowska, Lublin, Poland*
e-mail: mandziitaras@gmail.com

Two compounds $[Co(BG)_3]Fum\cdot1.5H_2O$ (**I**) and $[Ni(PG)_3]Fum\cdot H_2O$ (**II**), where: BG – benzohydrazide, PG – phenylacetic acid hydrazide and Fum – fumaric acid anion, were obtained and characterized by elemental analysis, X-ray diffraction and IR-spectroscopy.

Fumaric acid anion is a part of complexes in the form of a double-charged outer-sphere anion. In the case of the complexes described, the coordination polyhedrons are constructed of metal atoms coordinated by three ligand molecules that are deployed according to the "screw" rule regardless of its nature. Crystallization water molecules are also present in the structure.



I



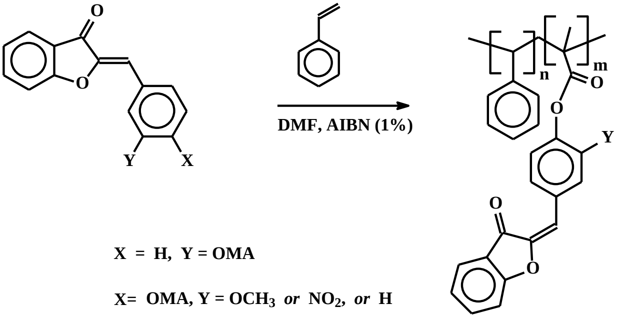
II

EFFECT OF ADDITION OF THE MONOMERS BASED ON 4′-METHACRYLOXYAURONES ON THERMAL STABILIZATION OF POLYSTHYRENE.

A. Martynes-Harsiia, N. Iukhymenko, A. Kolendo
Department of Macromolecular Chemistry, Taras Shevchenko National University of Kyiv, 60 Volodymyrska Street, Kyiv, Ukraine, 01033
e-mail: yukhimenko.n@gmail.com

The question of thermostability of polymers and the search for ways to increase it is always possible, because they arise at each stage of the existence of polymeric materials - in their production and storage, in the processing of products and further use. Research on the aging and stabilization of polymers, in particular polystyrene (PS), which is widely used in various industries, is an urgent task and has a practical focus on finding new efficient and relatively inexpensive stabilizers.

To create such polymers, we have synthesized new methacrylic monomers based on aurons.



X = H, Y = OMA

X= OMA, Y = OCH_3 *or* NO_2, *or* H

Polystyrene and modified samples were synthesized by free radical polymerization according to well-known method. The polymerization was carried out in 10 wt% DMF solution of monomers and was conducted using azobis(isobutyronitrile) (AIBN) as a free-radical initiator (1 wt% of monomer) at 78°C for 16 h in a solution of ethyl acetate, in an argon atmosphere.

The intra-chain stabilizing effect of auron derivatives, on the destruction of polystyrene, has been investigated. It has been established that the applications studied additives with covalent introduction significantly inhibit the process of its degradation in comparison with industrial polystyrene produced by Styron (Switzerland).

DESIGN, SYNTHESIS AND INVESTIGATION OF 1,8-NAPHTHALIMIDE BASED COMPOUNDS

Naveen Masimukku[a], Dalius Gudeika[a], Dmytro Volyniuk[a], Juozas Vidas Grazulevicius[a]
[a] *Kaunas University of Technology, Department of Polymer Chemistry and technology, Radvilenu plentas 19, LT-50254, Kaunas, Lithuania*
naveen.masimukku@ktu.edu

Development of orange red thermally-activated-delayed-fluorescence (TADF) emitters has been lagging behind when compared with blue and green fluorophores. TADF occurs due to reverse intersystem crossing. It is possible when the energy difference between excited singlet (S_1) and triplet (T_1) energy levels is very low [1]. External quantum effiencies (EQEs) of TADF OLEDs have been rapidly boosting in past few years The most efficient red TADF-OLED reported to date, based on a heptaazaphenalene derivative, has a state-of-the-art EQE of 17.5% with an EL emission maximum (λ_{EL}) at ≈610 nm and CIE coordinates of (0.60, 0.40). However, there is still much room for improving the overall performance due to poor color purity and significant roll-off at high current density. Thus, further developing high-performance pure-red TADF materials and their devices with CIE coordinates close to the National Television System Committee (NTSC) standard red (0.67, 0.33) is a key challenge for OLED technology. However, the highest EQEs of orange–red TADF OLEDs are significantly lower compared to those of blue and green TADF OLEDs [2].

Four 1,8-naphthalimide based compounds were synthesized. The synthesis of these compounds was carried out in three steps. It included bromination, imidazation and Buchwald-Hartwig coupling. The structures of the synthesized compounds were confirmed by nuclear magnetic resonance spectroscopy and mass spectrometry. Photophysical, electrochemical, thermal properties and performance in OLEDs will be reported.

Acknowledgements

This project has received funding from the Research Council of Lithuania agreement No [S-LU-20-3].

References

[1] Jia-Xiong. Chen, Wen-Wen. Tao, Ya-Fang. Xiao, Kai. Wang, Ming. Zhang, Xiao-Chun. Fan, Wen-Cheng. Chen, Jia. Yu, Shengliang. Li, Feng-Xia. Geng, Xiao-Hong. Zhang, and Chun-Sing. Lee, *ACS Applied Materials & Interfaces*, **2019**, *11* (32), 29086-29093.

[2] You-Jun. Yu, Xun. TangHui, Ting. Ge, Yi. Yuan, Zuo-Quan. Jiang, Liang-Sheng. Liao, *Organic Electronics*, ***2019***, *73*, 240-246.

NANOSIZED Pt-SnO$_2$ GAS SENSITIVE MATERIALS FOR CREATION SEMICONDUCTOR SENSORS TO HYDROGEN

Matushko I.P., Oleksenko L.P., Maksymovych N.P., Lutsenko L.V., Fedorenko G.V.
Chemical Department, Taras Shevchenko National University of Kyiv,
64 Volodymyrs'ka Str., Kyiv 01601, Ukraine
e-mail: mipigor@gmail.com

It's known that hydrogen is the cleanest fuel and promising ecological industrial energy source. But H_2 is a very explosive gas that's why it is necessary to control its leakage in air during production, storage, transportation and usage of hydrogen. Adsorption semiconductor sensors can be used to determine H_2 content. Development of new nanosized materials for the sensitive layer of the sensors is necessary to increase their H_2 sensitivities that is an actual task nowadays. Besides, significant increasing the sensitivities of the sensors can be also achieved by introduction of catalytic active additives to the gas sensitive material of the sensor. It is known that platinum is a promising for this goal because it is a very active catalyst of H_2 oxidation reaction. The aim of the work was to obtain Pt/SnO$_2$ sensor nanomaterials and study their morphology, catalytic and gas sensitive properties.

Nanosized material SnO$_2$ was prepared by a sol-gel method. Introduction of the platinum additives to the nanomaterial was performed by impregnating it with H_2PtCl_6 solutions of different concentrations ($0.84 \cdot 10^{-2}$ – $35 \cdot 10^{-2}$ M). The adsorption semiconductor sensors were made by thick film technology and their gas sensitive properties were studied. A ratio of the electrical resistance of the sensor in air (R_0) to its electrical resistance in the analyzed gas with concentration of 40 ppm H_2 in air (R_g) was chosen as a measure of the sensor response ($\gamma = R_0/R_g$).

To investigate phase composition and morphology of Pt/SnO$_2$ based materials TEM and XRD analysis were performed. It was shown that particle sizes of SnO$_2$ nanomaterial ranged from 5 to 30 nm (an average particle size was 17 nm) and the structures of the samples correspond to a cassiterite. It was found that reflexes which belong to Pt^0 were presented in diffraction patterns of Pt-containing SnO$_2$ materials obtained with solutions of H_2PtCL_6 starting from $10.6 \cdot 10^{-2}$ M concentration. Presence of the metallic platinum particles in these samples agrees with the results of diffuse reflectance spectroscopy that showed a wide absorbance band at 350–550 nm which can be attributed to plasma resonance absorption of the Pt nanoparticles. It was found that the obtained Pt-containing materials possessed high catalytic activities in H_2 oxidation reaction. Study of the sensors based on the obtained Pt/SnO$_2$ nanomaterials was shown that usage of the nanosized materials and introduction of Pt increased their sensitivities greatly. The highest sensor response to H_2 was found for the sensor obtained by impregnation of the nanosized SnO$_2$ with a solution of $15 \cdot 10^{-2}$ M H_2PtCl_6 concentration at the sensor heater power consumption of 0.25 W.

RESEARCH OF MORPHOLOGY OF WORKING SURFACES OF CONTACTS AND PHYSICAL MECHANICAL PROPERTIES OF ECOLOGICALLY SAFE ELECTRIC CONTACT MATERIALS

Korobsky V.V., Mrachkovsky A.M.,
National University of Life and Environmental Sciences of Ukraine,
st. Heroes of Defense, 12, Kyiv, 03041, Ukraine
e-mail: kor.vladlen.2002@gmail.com

Abstract. The results of studying the morphology of the working surfaces of the contacts of electrical devices using a Cambridge Stereoscan S4-10 scanning electron microscope with an attachment for X-ray spectral analysis Link System - 290 and X-ray microanalyzers "Camebax SX - 50" are presented. The laws of physical and mechanical processes occurring during restoration of the contact surface of electromagnetic starters, relays are revealed.

It is noted that the restoration of contacts of switching devices by coating the worn working layer with the electrospark method and gas-plasma spraying are the simplest, economically feasible ways to restore devices.

Key words: electric apparatus, contact system, ecologically safe composite material, metal-ceramic contact, electrical conductivity.

Research results. The reliability of the electrical contact is mainly determined by its constituent components, the structure and properties of the surface layers, which are formed as a result of erosion and transfer of contact material in an electric arc. The main component for serial contact materials of common electromagnetic starters and relays is silver. We have created environmentally friendly contact materials based on copper with impurities.

A metallographic analysis of the working surfaces of composite contacts contributed to the identification of the patterns of electroerosive destruction of explosive bridge contacts based on Ag and Cu, the establishment of the causes that cause one or another type of erosive destruction of contacting surfaces. Erosion wear of breaking contacts can be caused by the presence of erosion bridges, the action of a short arc (mass transfer from the anode to the cathode), the appearance of a plasma arc (predominant mass transfer from the cathode to the anode). A distinctive morphological feature of the impression of a plasma arc is a significant difference in the sizes of the cathode ($\alpha_{к}$) and anode spots (α_{a}) that remain on the surface of the contacts and it should be noted that $\alpha_{a} < \alpha_{к}$, while for a short arc is characteristic $\alpha_{a} = \alpha_{к}$. The X-ray spectral analysis of the contacts makes it possible to study the influence of arc energy on the distribution of the phases of the components in the surface layers.

When restoring the working layer of the contacts, materials were taken for comparing the physicomechanical properties: copper, brass, aluminum, and COK15 material. The following physical and mechanical properties were determined during the study: stiffness during switching tests, density of sprayed materials, coating porosity, fatigue strength of sprayed materials, determination of coating thickness.

RESEARCH OF THE PHASE COMPOSITION OF AUTOCLAVE AND NON-AUTOCLAVE AERATED CONCRETE CONTAINING FERROSILICON AS A GASIFIER

A.O. Musina, O.O. Sihunov, T.V. Kravchenko, A.O. Hura
Ukrainian State University of Chemical Technology,
Avenue Gagarina 8, Dnipro, 49005, Ukraine
e-mail: musinka.alinka19@ukr.net

Aerated concrete is by far the most sought after material in the construction market. It combines high thermal insulation and structural properties. The properties and durability of aerated concrete depend to a large extent on the quality of the structure.

The phase composition of non-autoclave and autoclave aerated concrete, which contains ferrosilicon as a gasifier, was researched using X-ray method. The identification of XRF peaks was performed using the reference data given in [1].

X-ray analysis showed that the researched samples of non-autoclave aerated concrete contain tobermorite of 11.3 Å ($5CaO{\cdot}6SiO_2{\cdot}5.5H_2O$), xonotlite ($6CaO{\cdot}6SiO_2{\cdot}H_2O$) and α-hydrate of dicalcium silicate ($2CaO{\cdot}SiO_2{\cdot}H_2O$). According to X-ray phase analysis, it is established that in the autoclave hardening samples at elevated temperature the tobermorite is not identified at autoclave treatment temperature, possibly it is converted to xonotlite ($6CaO{\cdot}6SiO_2{\cdot}H_2O$), and also α-hydrate of dicalcium silicate ($2CaO{\cdot}SiO_2{\cdot}H_2O$) at sufficiently high temperatures partially converts to hillebrandite ($2CaO{\cdot}SiO_2{\cdot}1.17H_2O$).

Additionally, peaks of hyrolite can be seen on radiographs of autoclaved aerated concrete. The small amount of this calcium hydrosilicate is explained by the fact that its formation occurs very slowly, possibly because it takes place at the point of contact of the quartz grains and tobermorite. It should be noted that for non-autoclave and autoclave aerated concrete the most intense are peaks 3.29-3.32 Å, which are characteristic of quartz.

The obtained results of the determination of the phase composition of the products of hydration of aerated concrete are confirmed by the data presented in studies [2].

Therefore, by means of X-ray phase analysis method, it was possible to investigate the phase composition of aerated concrete under different conditions of hardening, which contains ferrosilicon as a gasifier and to establish the presence of the main products of hydration.

[1] Gorshkov V.S., Timashev V.V., Sveliev V.G., Methods of physicochemical analysis of binders. Moscow, Vysshaya shkola Publ., 1981, p. 335

[2] Musina A.O., Sihunov O.O., Kravchenko T.V., Hura A.O., Features of thermodynamic analysis of reactions in the system FeSi – $Ca(OH)_2$ – H_2O and $FeSi_2$ – $Ca(OH)_2$ – H_2O., Voprosy Khimii i Khimicheskoi Tekhnologii., 2019, No. 6, p. 136-143

INFLUENCE OF THE METHOD OF OBTAINING GAS SENSITIVE MATERIALS ON CHARACTERISTICS OF CO-CONTAINING SENSORS CREATED ON THEIR BASE

Matushko I.P., Maksymovych N.P., Oleksenko L.P., Scolyar G.I., Ripko O.P.
Chemical Department, Taras Shevchenko National University of Kyiv,
64 Volodymyrs’ka Str., Kyiv 01601, Ukraine
e-mail: mipigor@gmail.com

Adsorption-semiconductor sensors based on metal oxides are widely used to determine the presence of toxic and explosive gases in the ambient air. High sensitivity of the such sensors, good dynamics of the response to an analyzed gas, small masses and dimensions, low power consumptions make them indispensable when creating small-sized, relatively cheap gas-analytical devices. The principle of the adsorption-semiconductor sensor operation is based on a change in an electrical resistance of its gas-sensitive layer in the presence of the analyzed gas.

Chemical composition of the material of this layer and its morphology significantly affect the electronic processes that determine the sensitivities of the sensors to the gases. Usage of the nanomaterials as gas sensitive layers of the sensors are promising for increasing the sensitivities of the sensors in comparison with usage of microcrystalline materials for the same goals.

In our work to create the nanosized material a non-aqueous sol-gel method was used. It allowed to obtain tin dioxide nanomaterial with antimony additives with particles of very small sizes (an average size of 12 nm). The usage of ethylene glycol as a solvent in this method also ensured its action as a hydrolytic agent which provides formation of the corresponding glycolates of tin (IV) and antimony (III). Increase in the temperature in the process of the nanoscale material sythesis the polymerization of the obtained glycolates leads to the creation of a three-dimensional grid where ethylene glycol molecules act as bridges between tin and antimony atoms. This structure-forming function contributed to the practical absence of agglomeration of the particles of the material during heat treatment of the xerogel, that prevented increasing the sizes of its particles. In order to increase the sensitivity of the sensors, cobalt oxide, a known catalyst for hydrogen oxidation, was added to the resulting material.

Comparison of the gas sensitive properties of the hydrogen sensors based on semiconductor materials of the same composition ($Co_3O_4/SnO_2/Sb_2O_5$) with the particle size of 1-30 μm obtained by the method of co-precipitation of hydroxides of tin and stybium obtained from their chlorides and the same material with the particle size of 5-25 nm obtained by the sol-gel method was done in the work.

It was found that the sensor based on nanoscale $Co_3O_4/SnO_2/Sb_2O_5$ material was more sensitive to H_2: its electrical resistance had changed in 13.9 times in the presence of 500 ppm H_2 compared to the analogous but microcrystalline sensor (the elecrical resistance of this sensor had only changed in 6.2 times). Explanation of the improved characteristics of sensors based on nanoscale material by the influence of its morphology on the electronic processes running on the surface of the sensor was done in the work.

BENZOPHENONE PHENOTHIAZINE-5,5-DIOXIDE MATERIAL EXHIBITING PHOTO-INDUCED CONFORMATIONAL REARRANGEMENTS

Edgaras Narbutaitis[a], Matas Guzauskas[a], Dmytro Volyniuk[a], Juozas Vidas Grazulevicius[a]
[a] *Kaunas University of Technology, Department of Polymer Chemistry and Technology,*
Radvilenu pl. 19, LT-50254, Kaunas, Lithuania
e-mail: edgaras.narbutaitis@ktu.edu

Organic light-emitting devices (OLEDs) have garnered much attention in recent decades, much of the effort has been spent developing materials which utilize both singlet and triplet excitons to attain high quantum efficiencies of the devices. Many of these materials are based on all-organic frameworks exhibiting thermally-activated delayed fluorescence (TADF) phenomena first demonstrated by Adachi et al. [2].

In this work we present novel multi-functional organic material PTZDO-BP which exhibits both TADF properties and conformational rearrangements induced by UV irradiation in solution. Due to these surprisingly irreversible physical changes in solution, the material exhibits linear response to UV irradiation intensity enabling it to be utilized as UV dosimeter.

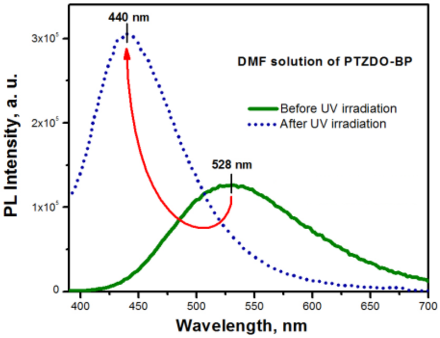


Figure 1. Photoluminescence spectra of PTZDO-BP before and after UV irradiation

Acknowledgements. This work was supported by the Research Council of Lithuania within scientific co-operation program between Lithuania and Ukraine ("LUW", S-LU-20-9).

[1] L. Xiao, Z. Chen, B. Qu, J. Luo, S. Kong, Q. Gong, J. Kido, Recent Progresses on Materials for Electrophosphorescent Organic Light-Emitting Devices, *Adv. Mater.*, **2011**, 23, 926-952.
[2] H. Uoyama, K. Goushi, K. Shizu, H. Nomura, C. Adachi, Highly Efficient Organic Light-Emitting Diodes from Delayed Fluorescence, *Nature*, **2012**, 492, 234-238.

THIN NANOPOROUS GRAPHITIC FILMS FABRICATED BY MAGNETRON PLASMA CHEMICAL VAPORE DEPOSITION FROM ACETYLENE

A.Nazarov[a], O.Slobodian[a], A.Rusavsky[a], Yu.V.Gomeniuk[a], N.Pavlusiak[b], A.Vasin,[a]
T.Nazarova[b], O.Gudymenko[a], O.Khyzhun[c], V.Stepanov[a], D.Kisyl[a]
[a] *Lashkaryov Institute of Semiconductor Physics NASU, pr. Nauky 41, 03028 Kyiv, Ukraine*
[b] *National Technical University “Igor Sikorsky KPI”, pr. Peremogy 37, 03056 Kyiv, Ukraine*
[c] *Frantsevych Institute for Problems of Materials Science NASU, str. Krzhizhanovsky 3, 03142 Kyiv, Ukraine*
e-mail: nazarov@lab15.kiev.ua

Carbon nanoporous thin films are very attractive for application in fields of supercapacitors, fuel cells, gas sensors and others. However due to their high resistance an employment of this material for resistance gas sensor is problematic. In our previous paper [1] it was proposed a new method of the porous carbon films deposition named as Magnetron Plasma Enhanced Chemical Vapour Deposition (MPECVD), where argon-methane gas mixture was used as active gas. However, after annealing at 650ºC, which resulted in strong graphitization of the film, a porosity of the films was decreased and the film resistivity was not enough small. In this work for increasing of porosity of the carbon film and obtaining low resistance an employment of argon-acetylene gas mixture is proposed. A comparative study of transformation of nanoporous carbon film produced in different carbon-hydrogen atmosphere into graphitic one, their structural and electrical properties are presented. The films of nanoporous carbon were fabricated on silicon or SiO_2/Si wafers. To clarify chemical structure of the film FTIR spectroscopy and XPS were used. X-ray refraction (XRR) method allows us to determine a density and a thickness of the films. Four-point probe method and transmittance line (TSL) technique were used for the analysis of electrical properties. Additionally, electrical conductivity at different temperature and frequency was examined by measurement of resistance between two nearest Ni contacts.

It was shown that initial deposited films have mainly sp^3 C-H bonds without appearance of silicon bonds. A density of the films was about 1.3 g/cm^3 for both carbon films that corresponds to nanoporous carbon, resistivity was about 10^8 Ohm×cm. After thermal annealing at 650°C for 30 min in N_2 atmosphere the sp^3 C-H bonds are disappeared, and C=C sp^2 bonds are formed. Besides the resistivity the films synthesized in argon-methane gas mixture decreases to 10^4 Ohm×cm whereas the films synthesized in argon-acetylene gas mixture decreases their resistivity up to 10^2 Ohm×cm. The density of the C films synthesized in in argon-acetylene gas mixture falls to 1.01 g/cm^3 that corresponds to 55% of porosity. It was shown that using of acetylene gave us a possibility to change a structure and electrical properties over a wide range in dependence on the film deposition regimes.

[1] O.M.Slobodian et all., *Applied Surface Science*, **2019**, 496, 143735(1-9).

MOLECULAR RELAXATIONS IN MODIFIED MICROCRYSTALLINE CELLULOSE

Alekseev O.[1], Lazarenko M.[1], Nedilko S.G.[1], Revo S.[1], Scherbatskii V.[1], Teselko P.[1], Prokopets V.[1]. Hamamda S.[2], Dorbani T.[2], Naoui Y.[2], Boyko V.[3], Sheludko V.[4], Gomenyuk O.[4]

[1] *Taras Shevchenko National University of Kyiv, 64/13 Volodymyrska str., 01601 Kyiv, Ukraine;*

[2]*Laboratory of Thermodynamics and Surface Treatment of Materials, University of Frères Mentouri Constantine 1, B.P. 325 Route Ain El Bey, Constantine 25017, Algeria*

[3]*National University of Life and Environmental Sciences of Ukraine, 15 Geroiv Oborony st., 03041, Kyiv, Ukraine*

[4]*Oleksandr Dovzhenko Hlukhiv National Pedagogical University, 24 Kyjevo-Moskovs'ka st. 41400, Hlukhiv, Ukraine*

The microcrystalline cellulose (MCC) has become increasingly popular lately among the structural modifications of cellulose, as it has a structure and properties that distinguish it from traditional fibrous or powdered cellulosic materials. Cellulose and its derivatives are characterized by several thermally initiated relaxation and phase transitions. Water and various impurities, in particular inorganic ones, which are in the MCC affect the mobility of cellulose molecules, the characteristics of the noted transitions and their manifestation in the properties of the MCC. In addition, the movement of cellulose molecules is different in its crystalline and amorphous parts, as well as in the intermediate layers.

It is believed that the relaxation of the excited states of the cellulose molecules may be related to the movement of methylol groups, or to the movement of cellulose chain segments, the latter being less likely for crystalline phase molecules compared to amorphous ones. At the same time, the movement of methylol groups on the surface of crystallites is quite possible. In order to clarify the role of these mechanisms, we have conducted a complex study of both “pure” MCC and that one containing different amounts of moisture and MCC filled with micro/nanoscale particles of inorganic dielectric oxides. In some cases, such particles played the role of luminescent probes, as they were activated by luminescent ions of rare earth or transition elements. To study the peculiarities of the molecules motion of and their relation to the structure and morphology of MCC the methods of X-ray diffraction, electron and optical microscopy, dilatometry, calorimetry, thermogravimetry, dielectric spectroscopy; vibration - IR, electron -vibration and luminescence spectroscopy were applied. The characteristics of the MCC samples were studied in the temperature range of -150 - 200 ^{0}C. The temperature dependences of the real and imaginary parts of the complex dielectric constant were studied at the frequencies of the applied electromagnetic field of 5, 10, 20, and 50 kHz. Comparison of experimental results and model estimations revealed the important role of conformational tg↔gt reorientation of the methylol groups in low-temperature relaxation processes in the MCC. It has also been shown that glycosidic bonds between glucose rings in cellulose molecules and primary hydroxyl groups do not participate in conformational movement in the range of the MCC dielectric relaxation. The conclusion was made that oxide particles block the movement of the methylol groups or bind all the water molecules leaving the MCC molecules free of the hydration shell. The obtained results confirmed the validity of the proposed models and showed the prospects of practical use of the composite systems such as “MCC – oxide”.

FLUORESCENCE PROPERTIES INTERACTION INTERFERON A2B WITH OLIGO- AND MONORIBONUCLEOTIDES

R.O. Nikolaiev, Ye.Yu. Stepanenko, S.I. Chernykh, Z. Yu. Tkachuk
[1] *Institute of Molecular Biology and Genetics of NASU, 150, Ac. Zabolotnogo St., Kyiv, Ukraine, 03680*
e-mail: romanfromukrain@gmail.com

Oligonucleotides antiviral drugs have actively used in medicine over the last decades, but the molecular mechanism of their action remains unclear. The RNA-based drug is known to increase interferon production and stimulate nonspecific antiviral protection. As shown in our previous works, the combination of oligonucleotides with alcoholic sugar with D-mannitol leads to changes in their biological activity and efficiency.

In our study, we studied the interactions of mononucleotides (NMP), yeast oligoribonucleotides (ORNs), their Na^+ salts (ORNsNa), and complex with D-mannitol (ORNs-D-M) with Interferon α2b – a key protein of the antiviral cell defense mechanism. To investigate the interaction mono- and oligonucleotides with IFN, the fluorescence spectroscopy and quenching time of fluorescence used.

Thus, when using the ORNs and ORNs:D-M, quenching of fluorescence INF was 25% and 28%, AMP and AMP:D-M – 15 and 21%, GMP and GMP:D-M – 32% and 45%, CMP and CMP:D-M – 38% and 42%, UMP and UMP:D-M - 13% and 14%. The quenching of fluorescence INF when titrated ORNsNa and ORNsNa:D-M was 16% and 17%, AMPNa and AMPNa:D-M - 8% and 10%, GMPNa and GMPNa:D-M - 8% and 16%, CMPNa and CMPNa:D-M - 11% and 18%, UMPNa and UMPNa:D-M - 11% and 12%.

INF has a lifetime of 2.95 ns. When interacting with ORNs and ORNs:D-M INF has a fluorescence lifetime 2.37 and 2.32 ns, respectively, AMP and AMP: D-M 2.01 and 1.92 ns. GMP and GMP: D-M 2.52 and 2.53 ns, CMP and CMP: D-M 2.28 and 2.24ns, UMP and UMP: D-M 2.56 and 2.25 ns. When interacting with ORNsNa and ORNsNa:D-M INF has a fluorescence lifetime of 2.73 and 2.49 ns, respectively, AMPNa and AMPNa: D-M 2.31 and 2.43 ns. GMPNa and GMPNa: D-M 2.58 and 2.61 ns, CMPNa and CMPNa: D-M 2.87 and 2.68 ns, UMPNa and UMPNa: D-M 2.8 and 2.7 ns. The most active quenching of fluorescence obtained using acid forms in combination with mannitol.

Thus, we assume the same compound in various forms may act as an inhibitor and activator for the protein. To test this assumption in the case of nucleotide ligands, we plan to conduct studies with the interferon receptor. The ribonucleotides have the advantage of interacting with proteins, unlike salt form, because they have a stronger binding. Various binding sites can explain different effects of different forms of NMPs on the fluorescence properties of the INF.

NEW PARAMAGNETIC CENTER IN Cu-DOPED Y-STABILIZED ZrO_2

V.V. Nosenko[1,2*], I.P. Vorona[1], S.M. Okulov[1], L.Yu. Khomenkova[1,2], N.O. Korsunska[1]
[1]*V. Lashkaryov Institute of Semiconductor Physics of NAS of Ukraine, 45 pr. Nauky, 03028 Kyiv, Ukraine*
[2]*National University «Kyiv-Mohyla Academy», 2 Skovorody str., 04070 Kyiv, Ukraine*
e-mail: vvnosenko@ukr.net

Cu-doped ZrO_2 composites have been intensively investigated in recent years due to their excellent properties offering diverse applications such as high temperature and corrosion resistant coatings, oxygen sensors, radiation detectors, biological labelling, catalysts etc. The properties of such composite depend mainly on Cu spatial localization. In addition, Cu-doping stimulates an appearance of a specific photoluminescence (PL) in green spectral range that can offer optical applications.

Electron paramagnetic resonance (EPR) is a proper method for investigation of Cu-related centers in ZrO_2 matrix. Combination of this technique with the investigation of light emitting properties allows clarifying the role of these centers in the emission processes.

Here, we report the EPR results of Cu-doped Y-stabilized ZrO_2 powders calcined at 800-1000°C. It was found that the calcination of the samples at high temperatures leads to dramatic modification of EPR spectrum and appearance of new Cu-related signal. Computer simulations of both X- and Q-band spectra allowed to determine the following parameters of the copper centers: S=1/2, I=3/2, g_x=2.021, g_y=2.026, g_z=2.168, $A_{xx}\sim40\times10^{-4}$ cm^{-4}, $A_{yy}\sim35\times10^{-4}$ cm^{-4}, $A_{zz}\sim186\times10^{-4}$ cm^{-4}, $A_{xz}\sim10\times10^{-4}$ cm^{-4}, $A_{yz}\sim5\times10^{-4}$ cm^{-4} for the ^{63}Cu isotope (for ^{65}Cu the hyperfine constants should be multiply by 1.07). The analysis of the experimental data allows proposing center model as Cu_{Zr}^{2+} in the monoclinic ZrO_2 lattice.

These Cu-related EPR centers are also responsible for specific green-yellow PL bands. This conclusion was confirmed by simultaneous decrease of corresponding EPR and PL signal intensity observed for the powders submitted to quenching after calcination. This decrease was caused by the Cu ions out-diffusion and formation of CuO phase on the grain surface, which results in the increase of CuO-realted absorption band.

SYNTHESIS AND CHARACTERIZATION OF A NEW $Sn_{1-x}Mn_xBi_2Te_4$ SOLID SOLUTIONS AS A POTENTIAL MAGNETİC TOPOLOGICAL INSULATORS

E.N. Orujlu[a], Z.S. Aliev[b], M.B. Babanly[a]
[a] *Institute of Catalysis and Inorganic Chemistry, ANAS, Baku, AZ 1143, Azerbaijan*
[b]*Azerbaijan State Oil and Industry University, Baku, Azerbaijan*
elnur.oruclu@yahoo.com

Layered tetradymite type structured chalcogenides are desirable novel materials for the future development of low-power electronic and spintronic devices [1-3]. Doping van der Waals layered materials with magnetic impurities which could induce novel exotic phenomena have been a subject of intensive studies lately.

In this paper, we investigate phase equilibria in the $SnBi_2Te_4$−$MnBi_2Te_4$ system since due to closeness of tin and manganese ionic radius there expected to have complete solid solubility which creates a chance to control desirable properties by adjusting the number of substitutional atoms.

The $Sn_{1-x}Mn_xBi_2Te_4$ compounds were synthesized using high purity elements (99,999 % purity from Alfa Aeser) in glassy carbon crucibles (avoid manganese side reactions) inside the quartz ampoules under vacuum condition at 700 ºC for 3 hours and additionally annealed at 450 ºC for ~ 500 h. The resulting ingots analyzed by differential thermal analysis (LINSEIS HDSC PT1600) and X-ray diffraction (Bruker D2 PHASER) methods.

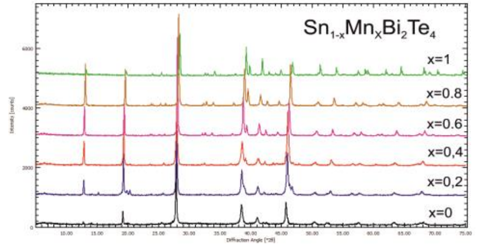


Figure. PXRD results of alloys

Fig. presents the PXRD patterns of some annealed $Sn_{1-x}Mn_xBi_2Te_4$ alloys. It is seen that each intermediate alloy has similar reflection lines with initial starting compounds belong to tetradymite-type hexagonal structure with space group *R-3m* (#166). Further, increasing x results of a slight shift of peaks to high angles which is characteristical for substitutional solid solutions. Both lattice parameters increase linearly with increasing concentration of Sn content according to Vegard’s law due to the larger radius of Sn^{2+} compared to Mn^{2+}. Based on DTA analysis and PXRD examinations the T-x diagram of the $SnBi_2Te_4$−$MnBi_2Te_4$ system was constructed. The system is non-quasi-binary due to the incongruent melting character of starting compounds, but it is stable below solidus and continuous solid solutions are formed in the whole composition range. Because of interaction between $SnBi_2Te_4$ and $MnBi_2Te_4$ is complex; phase equilibria above the solidus curve cannot be completed until the $SnTe$−$MnTe$−Bi_2Te_3 system fully studied.

[1]M.B. Babanly, et al., *Russ. J. Inorg.*, 2017, 62(13), 1703-1729.
[2]M.M. Otrokov, et al., *Nature*, 2019, 576, 416–422.
[3]R.S.K. Mong, et al., *Nature*, 2019, 576, 390-392.

EXCITATION DYNAMIC IN NEW TYPE DETECTORS BASED ON STILBENE

R. Karpicz[a], L.Valkunas[a], N. Ostapenko[b], Yu. Ostapenko[b] ,
O.Kerita[b], N. Galunov[c, d], I. Lazarev[d], Ya. Polupan[d]
[a] *Department of Molecular Compounds Physics, Center for Physical Sciences and Technology, Sauletekio Ave,9-111,10222, Vilnius, Lithuania, e-mail: leonas.valkunas@ff.vu.lt*
[b]*Institute of Physics of the NASU, 46, Prosp. Nauky, Kyiv, 03028, Ukraine, e-mail:*
e-mail: nina.ostapenko@gmail.com
[c]*Institute for Scintillation Materials of the NASU, 60, Prosp. Nauky, Kharkiv 61022, Ukraine*
[d]*V. N. Karasin Kharkiv National University, 4, Svobody Sq., Kharkiv, Ukraine*

New type of detectors for the ionized irradiation constructed by using polycrystals of hot pressing and composite scintillators of stilbene have the advantage over such devices based on stilbene monocrystals. The advantage of such detectors by using them in radioecology and radiomedicine is mainly due to lack of restriction of their size and configuration. Therefore, extended studies of the excitation dynamics in pressed and composite polycrystals of stilbene have been carried out by means of time-resolved fluorescence in broad temperature range, from 15 K up to room temperature. For comparison purpose the time-resolved fluorescence measurements have been also considered for the stilbene solutions in polystyrene and toluene.

Fluorescence spectra of polycrystals and composite scintillators demonstrate redistribution of the fluorescence intensity between different broad and narrow bands of the vibronic origin as well as the blue-shift of these bands by increasing the temperature. The shift of these vibronic bands reaches the value of 300 cm^{-1} or even more for the polycrystals. Since the stilbene molecule experiences the rotation of the benzene moieties connected by a flexible carbon bridge, distribution of multiple local states of the molecule should be inherent in the bulk material. These spectral changes are evidently due to the different population of the local states of higher energies with temperature.

In opposite of these observations, the fluorescence intensity of all bands of the stilbene solution decreases with temperature. Moreover, substantial differences are observed for the fluorescence lifetimes. In opposite to the well-known decay of the fluorescence lifetimes of the stilbene solutions with temperature, the lifetimes of the fluorescence of all bands of the polycrystals increases by increasing the temperature. Moreover, though in solutions the lifetimes of all bands are the same and vary between 1.18 ns up to 0.7 ns, the lifetimes of the fluorescence bands in polycrystals are larger for the bands of the longer wavelengths with changes between 1.5 ns and 2.8 ns. Model description of these phenomena cause by the polycrystallinity of stilbene will be presented.

HYBRID-CONTROLLED SYNTHESIS OF COBALT NANOPARTICLES IN AQUEOUS SOLUTIONS

N.M. Permyakova[a], T.B. Zheltonozhskaya[a], D.O. Klymchuk[b], V.V. Klepko[a],
L.N. Grishchenko[c], A.S. Fomenko[c], L.O. Vretik[c]
[a]*Institute of Macromolecular Chemistry, National Academy of Sciences of Ukraine,*
48 Kharkivske Shose, 02160 Kyiv, Ukraine
E-mail: permyakova@ukr.net
[b] *Institute of Botany, National Academy of Sciences of Ukraine, 2 Tereschenkovskaya St.,*
01601 Kyiv, Ukraine
[c]*Taras Shevchenko National University of Kyiv, Faculty of Chemistry,*
Department of Macromolecular Chemistry, 60 Volodimirska St., 01033 Kyiv, Ukraine,

In recent years, cobalt nananoparticles (CoNPs) have attracted considerable attention due to their outstanding magnetic properties as ferromagnetic materials, which use in high-density magnetic storage media, gene deliver and as targeted drug carrier. Well-developed CoNPs preparation methods, such as thermal decomposition, pyrolysis, plasma reduction of cobalt salts or their chemical reduction in polyol solutions, place high demands on equipment due to high temperatures, pressures or the use of organic solvents. This paper presents a simple and effective method for producing stable CoNPs in an aqueous medium using polymer/inorganic hybrid (PIH) based on silica nanoparticles and grafted polyacrylamide chains.

One sample of the hybrid was synthesized, carefully characterized, and used as a hydrophilic stabilizing matrix in the borohydride reduction of Co-salt. Using UV-Vis spectroscopy, TEM, and WAXS, we determined the kinetic parameters of the CoNP formation process as well as the yield, size, and morphology of nanoparticles in hybrid solutions and pure water at various concentrations of metal salt and hybrid. The growth of both concentrations had a positive effect on the rate of formation of metal nanoparticles and their yield, but in all cases the reduction process developed much slower in hybrid solutions compared to pure water. The morphology of the CoNPs/PIH composition is represented mainly by separate hybrid particles containing metal nanocrystals of ~1-7 nm in size (Figure)

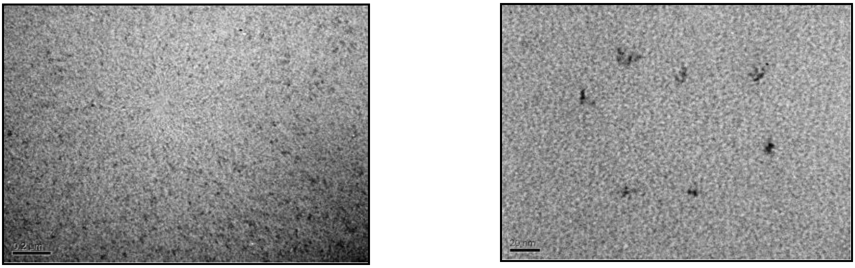


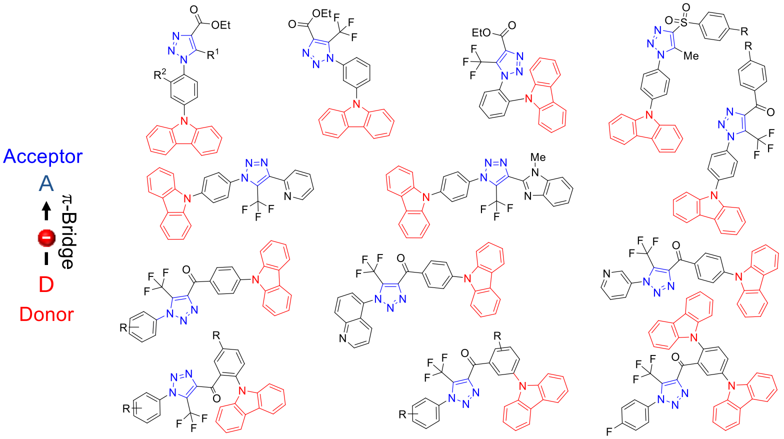
Figure – Real morphology of CoNPs synthesized in the PIH aqueous solutions.

NEW CARBAZOLE-π-BRIDGE-TRIAZOLE COMPOUNDS FOR OLED APPLICATIONS

N. Pokhodylo[1], R. Lytvyn[1], M. Stanicka[1], M. Tupychak[1], Kh. Pitkovych[1], O. Bezvikonnyi[2], E. Urbonas[2], D. Volyniuk[2], S. Kutsiy[3], K. Ivaniuk[3], V. Kinzhybalo[4], P. Stakhira[3], A. Tomkeviciene[2], J.V. Gražulevičius [2], M. Obushak[1]
[1]Ivan Franko National University of Lviv, Kyryla i Mefodiya 6, Lviv, Ukraine,
[2]Kaunas University of Technology, Baršausko 59, Kaunas, Lithuania
[3]National University “Lviv Polytechnic”, Stepan Bandera 12, Lviv, Ukraine.
[4]Institute of Low Temperature and Structure Research, Okólna 2, Wrocław, Poland
e-mail: pokhodylo@gmail.com

Within the last years, π-conjugated donor-acceptor (D-A) materials became the most widespread for exploration and use in the field of organic (opto)electronics. Application of such type compounds in OLEDs is based on the formation of intramolecular charge-transfer states under excitation, which confers them unique photophysical properties, including thermally activated delayed fluorescence, room temperature phosphorescence, piezoluminescence and etc. Consequently, synthesis and studies of new D-A compounds is an urgent task.

This presentation will highlight the design, synthesis, photophysical properties and OLED applications of new carbazole-triazole conjugates in which chromophores are linked through π-bridge in a different manner.



Acknowledgement: This research was financially supported by the Ministry of Education and Science of Ukraine and the Research Council of Lithuania within the framework of the bilateral program.

NEW CONDUCTING POLYMER NANOSTRUCTURED COMPOSITES FOR ECOLOGICAL MONITORING AND PROTECTION

A. Pud[a], N. Ogurtsov[a], M. Petrychuk[b], V. Oliynyk[b], V. Zagorodnii[b], O. Kruglyak[a]
[a] *V.P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry of NAS of Ukraine, 50 Kharkivske shose, Kyiv, 02160, Ukraine.*
[b] *Taras Shevchenko National University of Kyiv, Faculty of Radio Physics, Electronics and Computer Systems*
e-mail: alexander.pud@gmail.com; pud@bpci.kiev.ua

New conducting nanostructured hybrid composites of polyvinylidene fluoride (PVDF) and poly(3-methylthiophene) (P3MT) doped by plasticizing dodecylbenzenesulphonate (DBS), perfluorooctanoate and chlorine anions are synthesized for environmental (sensor) monitoring and electromagnetic interference (EMI) shielding. The kinetic features of the oxidative polymerization reaction of 3-methylthiophene (3MT) under the action of ferric chloride (III) in anhydrous medium without and in the presence of plasticizing dopants (DBS and PFO), as well as in the dispersions of PVDF submicron particles have been investigated.

The morphology of these composites has been studied. We find that unlike PVDF/P3MT-Cl in PVDF/P3MT-DBS nanocomposites, the P3MT phase additionally forms a thin layer of ~4 nm on the surface of PVDF particles. Such a structure indicates both sufficiently strong interphase interactions between the components and the core-shell morphology of the developed nanocomposites. Existence of these interactions is confirmed by the analysis of the FT-IR spectra of the nanocomposites which shows an increase of the π-conjugation length in the P3MT chains of the nanocomposite state compared to the pure polymer that matches well with their conductivity behavior. WAXD patterns of pure P3MT-DBS and its phase in the nanocomposites reveal crystalline reflexes of the hexagonal lattice. Analysis of these patterns shows that the oxidative polymerization of 3-methylthiophene in the presence of PVDF particles leads to an increased crystallinity of the P3MT-DBS phase in the nanocomposites. Specificity of this P3MT phase is confirmed also by its increased thermal stability as compared with the pure conducting polymer.

An influence of the doped P3MT content on the conductivity behavior of the nanocomposites has been investigated. In particular, it is found that the electrical conductivity of PVDF/P3MT-DBS nanocomposites significantly exceeds the electrical conductivity of PVDF/P3MT-Cl nanocomposites that is important for using these nanocomposites as materials for sensory measurements and absorption of electromagnetic radiation. The effects of the content of the electrically conducting polymer and the nature of the dopant both on the sensitivity of the formed nanostructured hybrid nanocomposites to vapors of VOC/ammonia and on EMI shielding effectiveness have been established.

A NEW OPERATING PRINCIPLE OF SELECTIVE DETECTION IN GASES

A.V. Savytskyi[a], G.V. Kamarchuk[a], A.P. Pospelov[b], A.O. Herus[a],
Yu.S. Doronin[a], V.L. Vakula[a], E. Faulques[c]
[a] *B. Verkin Institute for Low Temperature Physics & Engineering, 47 Nauky Ave., Kharkiv, 61103, Ukraine*
[b] *National Technical University "Kharkiv Polytechnic Institute", 2 Kyrpychov Str., Kharkiv, 61002, Ukraine*
[c] *Institut des Matériaux Jean Rouxel (IMN), Université de Nantes, CNRS, 2 rue de la Houssinière, BP 32229, 44322 Nantes cedex 3, France*
e-mail: savandrvlad@gmail.com

Diversity of operating principles implemented in modern sensor devices can be viewed as one of necessary prerequisites for a large-scale use of sensors in multifunctional technological cycles. We propose a new operating principle of selective detection in gases based on formation of an original quantum system and registration of its energy states in dynamic mode using dendritic Yanson point contacts. A quantum physical system can be characterized with a set of energy states (energy eigenstates) that correspond to a local minimum in the total energy of the system. Due to the quantum nature of their electric properties, Yanson point contacts are able to record minute variations in superficial states of the point contact conductivity channel which are caused by adsorption of an external agent during the cyclic switchover effect [1]. Energy parameters of the point-contact sensor response presented as a conductance histogram allow distinguishing materials one from another [2]. In the simplest case, the knowledge of the position of the main maximum in the conductance histogram is sufficient to determine the gas or liquid under analysis, because the positions of the conductance maxima in the histograms correspond to the most probable metastable states related to the specific cross sections of the dendritic Yanson point contacts synthesized in the self-oscillatory process.

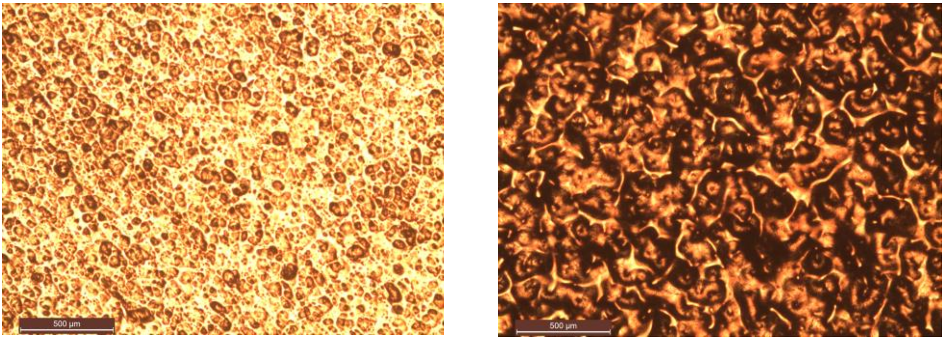
[1] A.P. Pospelov, A.I. Pilipenko, G.V. Kamarchuk, V.V. Fisun, I.K. Yanson, and E. Faulques, A new method for controlling the quantized growth of dendritic nanoscale point contacts via switchover and shell effects, *J. Phys. Chem. C,* **2015**, 119(1), 632-639.

[2] G.V. Kamarchuk, A.P. Pospelov, A.V. Savytskyi, A.O. Herus, Yu.S. Doronin, V.L. Vakula, E. Faulques, Conductance quantization as a new selective sensing mechanism in dendritic point contacts, *SN Applied Sciences,* **2019**, 1:244.

THE EFFECT OF BUTIL ALCOHOL ON ANODIC BRASS OXIDATION PROCESSES IN PHOSPHATE ELECTROLYTES

Silchenko D., Shkolnikova T., Pancheva H., Pilipenko A.
National Technical University «Kharkiv Polytechnic Institute», Kyrpyhova str. 2,
Kharkiv, 61002, Ukraine
e-mail: opilipenko1984@gmail.com

Electrochemical polishing (EP) is conducted to obtain a smooth defect-free metal surface. The essence of this method consists in that that the smoothing occurs due to the anodic dissolution of the surface layer of metal and the availability of the diffusion layer on the metal-electrolyte boundary results in the preferential dissolution of profile microelevations. The EP of copper alloys is carried out using phosphoric acid-based electrolytes with the addition of alcohols that display both inhibiting and surface-active properties.



а *б*

Fig. 1. The images of the surface of brass electrode after the anodic treatment in the phosphate-butanol solutions. The $C_4H_9OH:H_3PO_4$ ratio, volumetric fractions are 3:1(*a*) and 2:1(*b*). $j_a = 25\ A\cdot dm^{-2}$

The obtained research data allowed us to establish that the addition of butanol to the polishing electrolyte conditions an abrupt decrease in the current density in the studied potential range and inhibits the electrochemical brass dissolution. Butyl alcohol improves electrode surface wetting properties and ameliorates the metal working. The brass working quality depends on the content of alcohol in the electrolyte and the used current density (Fig.1). A better quality of treatment is observed in the solutions that contain 15 to 30 vol. % of butanol. However, the EP is accompanied by the removal of a large metal layer. An increase in the current density results in the worsened quality of surface treatment in the solutions with a high content of butanol. However, the effect of j_a is neutralized with a decrease in the alcohol content.

EFFECTS OF CHARGE ORDERING IN ELECTRONIC SUBSYSTEM OF QUASI-2D BEDT-TTF CONDUCTORS

Yu. Skorenkyy, O. Kramar, Yu. Dovhopyatyy
Ternopil Ivan Puluj National Technical University, 56 Ruska St, 46001 Ternopil, Ukraine
e-mail: skorenkyy@tntu.edu.ua

Diversity of electronic phases observed in low-dimensional organic conductors has become not only the fundamental theoretical problem [1], but also a premise of novel organic devices [2]. BEDT-TTF family of low-dimensional conductors exhibits large variety of transitions which are to be, and can be explained within the single model of electronic subsystem. To study the importance of specific electron-electron interaction terms of such a generic model, we focus on the interplay of the intersite Coulomb repulsion V, which induces charge ordering, and the correlated hopping of electrons, which causes peculiar dependence of energy characteristics on a doping [3]. By applying the projection method [4] in the Green function equation of motion approach we calculated the single-particle energy spectrum, sublattice magnetization in spin- and charge-ordered phases and the transition temperatures.

At different subband fillings the steepness of normalized Verwey temperature Θ_V/w (w stands for the unperturbed bandwidth) increase at rising V/w differs considerably and is the greater, the higher is the electron concentration. From one side, this allows effective control of Θ_V value by application of the external pressure which leadds to the decrease of V/w ratio, from the other side, in electric field composed of materials with charge ordering which have close values of n, in certain interval around intersection point of $\Theta_V(V/w)$ dependencies, in the contact region one can create a controlled transition from metallic (non-charge ordered) and insulating (charge-ordered) materials. Dependence of Θ_V on the band filling at different values V/w shows that intersite Coulomb correlation significantly influences the width of the concentration interval in which a charge order stabilizes. We attribute essentially different values of transition temperatures to differences of band gaps and different conductivities of materials with various V/w. In distinction from the greater-than-half-filled band, in the less-than-half-filled one the doping of cation subsystem can lead to sharp changes of conductivity related to the charge ordering stabilization. Increase of the correlated hopping parameter leads to the decrease of the critical value of electron concentration and increase of Verwey temperature in whole concentration interval of charge ordering stability.

[1] M. Dressel, *Crystals*, **2018**, 8, 332:1-3.
[2] F. Sawano et al, *Nature*, **2005**, 437, 522–524.
[3] Y. Skorenkyy, *Materials Today: Proceedings*, **2019,** doi.org/10.1016/j.matpr.2019.10.164.
[4] Y. Skorenkyy, O. Kramar, *Molecular Crystals and Liquid Crystals*, **2016**, 639, 24-32.

SYNTHESIS AND PHOTOLUMINESCENCE OF SILICA AND SILICA-TITANIA HYBRID MATERIALS DOPED WITH LANTHANIDE EDTA- AND DTPA-CHELATES

S.S. Smola, E.M. Fadieiev, N.V. Rusakova, I.V. Berezovskaya
A.V. Bogatsky Physico-Chemical Institute of the NAS of Ukraine, 86 Lyustdorfska doroga, Odesa, 65080, Ukraine
e-mail: sssmola@gmail.com

Lanthanide (Ln(III)) containing materials have generated great research interest in the past decade. Numerous studies in this area are concentrated on the development of novel applications in optoelectronic devices, solid state lasers, optical data storage and detectors due to narrow-band luminescence in a wide spectral range and large values of the excited states lifetime. The introduction of lanthanide complexes into hybrid materials minimizes the quenching of the Ln-centered emission, and, due to the significant concentration of emitting centers, high values of the luminescence intensity can be achieved.

Silica is the most used host in hybrid materials as it forms a thin network that can be used in terms of highly stable luminescent phosphors. On the other hand, titanium dioxide has excellent physical properties due to its high transparency in the visible region and good thermal characteristics. To our knowledge, it is rare that Eu (III) was added to SiO_2-TiO_2 composites, which can combine the outstanding optical properties of europium ions and hybrid inorganic hosts. In order to fully characterize these systems, we studied the influence of the Si : Ti ratio, the concentration of Eu(III) complex, and the order of addition of components on the emission properties of materials.

Present work highlights the results of spectroscopic studies of hybrid materials based on Eu(III) and Tb(III) chelates with complexones such as EDTA and DTPA embedded in silica and mixed inorganic SiO_2-TiO_2-matrices using both covalent and non-covalent interactions. Samples of different Si : Ti ratios as well as concentration of Ln(III) complexes were studied. The features of synthesis of such materials and the properties of lanthanide-centered luminescence in the visible region are discussed, as well as the perspectives of practical use.

SILVER DOPED TIO$_2$-LDH CLAY NANOCOMPOSITES FOR PHOTOCATALYTIC REDUCTION OF CARBON DIOXIDE

Starukh H.[a], Petryk I.[a], Koci K.[b]
[a] *Laboratory of Photonics Oxide Nanosystems, Chuiko Institute of Surface Chemistry, NAS of Ukraine, General Naumov's str 17, 03164, Kyiv, Ukraine*
[b] *Institute of Environmental Technology, VŠB-Technical University, 17 listopadu str, 15, Ostrava, 70800, Czech Republic*
e-mail: starukh_halyna@isc.gov.ua

Over the past a few decades, there have been growing interest to photocatalytic conversion of CO_2 due to the generating renewable hydrocarbon fuels that can be directly supplied to the energy infrastructure. The activity of researchers in the field of synthetic photosynthesis are focused on the search of efficient photocatalysts of CO_2 photoreduction offering high quantum yields, activity and selectivity. TiO_2 is the most widely used photocatalyst for the CO_2 reduction process due to its chemical stability, availability, low cost and anticorrosion properties [1]. The activity of TiO_2 depends on the type of crystalline phase, crystalline face, and the structure defects. However, the wide band gap of different TiO_2 types limits its application when irradiated with UV light since the solar spectrum only consists of about 4% of UV light. To increase the rate of methane, CO, methanol, ethane formation TiO_2 is combined with Pt, Au, Ag, Cu, etc. [2].

Layered double hydroxides (LDH), a class of ionic lamellar compounds or hydrotalcites, were reseantly reported as the alternative of semiconductor photocatalysts for renewable energy production [3]. For photocatalytic process of CO_2 reduction LDH could be especially attracted due to their relatively low cost, strong sorption capacity for CO_2, and the possibility to tune photocatalytic active sites and band gap by changing the metal cations in the layer structure. The application of LDH favors the CO_2 adsorption on the active sites of the photocatalysts that significantly influence the efficiency of CO_2 photoreduction proces.

The results on the synthesis and characterisation of silver-contained TiO_2-LDH nanocomposites will be presented. The activity of obtained materials with different content of silver and TiO_2 in photocatalytical process of CO_2 reduction will be compared.

[1] O. Ola, M. M. Maroto-Valer, Review of material design and reactor engineering on TiO_2 photocatalysis for CO_2 reduction. *J. Photochem. Photobiol. C*, 24, 2015, P. 16-42.

[2] Y. Izumi, Recent Advances (2012–2015) in the Photocatalytic Conversion of Carbon Dioxide to Fuels Using Solar Energy: Feasibilty for a New Energy in Jin et al.; *Advances in CO_2 Capture, Sequestration, and Conversion ACS Symposium Series*; American Chemical Society: Washington, DC, 2015. P. 1-46.

[3] Zhao, Y., Jia, X., Waterhouse, G. I.N., Wu, Li-Zhu, Tung, Chen-Ho, O'Hare, D., Zhang, T. Layered Double Hydroxide Nanostructured Photocatalysts for Renewable Energy Production. *Adv. Energy Mater.*, 6, 2016, 1501974.

INVESTIGATION OF MONTMORILLONITE INTERCALATION BY POLYVINYLPYRROLIDONE AND OBTAINING TERMOPLASTIC NANOCOMPOSITES

O. Suberlyak, V. Krasinskyi, O. Nikitchuk
Lviv Polytechnic National University, 12 Bandera str., Lviv 79013, Ukraine
e-mail: suberlak@polynet.lviv.ua

The aims of the work are:

- development of method for compatibility of montmorillonite (MMT) with water-soluble polymer – polyvinylpyrrolidone (PVP) – in order to use the obtained mixture for the modification of polar and non-polar polymers;
- investigation of structure and thermo-physical properties of montmorillonite-polyvinylpyrrolidone mixture (MPM), as well as efficiency of MMT intercalation;
- determination of modified montmorillonite effect on physico-mechanical, thermo-physical and insulating properties of polycaproamide PA-6.

A new method of layered silicate (montmorillonite) intercalation by polyvinylpyrrolidone in the solution under ultrasonic treatment is described in this work [1, 2]. The structure and thermophysical properties of the developed nanomodifier and the components rational ratio have been investigated [2]. The effect of intercalated montmorillonite on physico-mechanical, thermophysical and insulating properties of polycaproamide PA-6 has been determined [2, 3].

Thus, the experimental results confirm the positive effect of MPM in the composite with PA-6, allow to determine the rational composition of nanomodifier for polymers based on montmorillonite modified by polyvinylpyrrolidone at PVP:MMT ratio of 5:1 and confirm its efficiency while obtaining composites on the basis of polyamide-6 and MPM in the melt. The introduction of the developed MPM into polyamide in small amounts significantly improves its mechanical, thermophysical and insulating properties but reduces its elasticity. Therefore, the developed composites based on PA-6 with filler may be recommended for the production of construction materials with increased hardness and strength.

[1] Krasinskyi V., Suberlyak O., Zemke V., Klym Y., Gaidos I. *Chemistry & Chemical Technology*, **2019**, 13 (1), 59-63.

[2] Krasinskyi V., Suberlyak O., Dulebová L. and Antoniuk V. *Key Engineering Materials*, **2017**, 756, 3-10.

[3] Krasinskyi V., Kochubei V., Klym Yu., Suberlyak O. *Eastern-European Journal of Enterprise Technologies*, **2017**, 4 12 (88), 44-50.

SOME FEATURES OF EFFECTIVE STACKING INTERACTIONS IN AROMATIC POLYAMIDES

A.V. Tokar, O.P. Chigvintseva
Dnipro State University of Agriculture and Economics
25, S. Yefremov St., Dnipro, 49600, Ukraine
e-mail: atokar_2004@ukr.net

Stacking interactions are well known as to be predominantly non-valent intermolecular interactions that occur between π-aromatic fragment systems and have the nature of weak Van-der-Waals bonds. Such interactions, along with "classical" hydrogen bonding, play an important role in shaping the structure of aramid polymeric materials, in particular phenylons.

Investigation of the electron density distribution in model supermolecules of benzene dimers (Fig. 1) with T-shaped, parallel-displaced and sandwich structures *in vacuo* shows that the first two types of dimers correspond to the minima on the surface of potential energy, and the structure with parallel-displaced molecules is more stable, while the sandwich one is in transition between them [1–3].

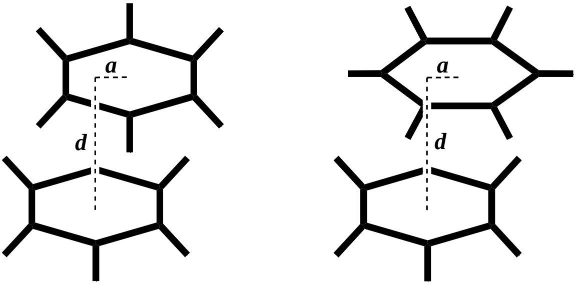


Fig. 1. Examples of some conformations of the benzene dimer with the parameters of π-stacking interactions

In the case of the dimerized form of the model compound N-phenylbenzamide, which reproduces the peculiarities of the hydrogen bonding effects in the polymer phenylon matrix, the separation of the obtained equilibrium dimer geometry into the monomer components with their further optimization is approximated by B3LYP/6-311++G(d,p) led to the formation of two identical structures. The calculation of vibrational frequencies for all localized stationary points showed the absence of imaginary vibrations, which made it possible to characterize them as minima on the surface of potential energy.

[1] P. Munshi, *CrystEngComm.*, **2005**, 608-611.

[2] O. Zhikol, *J. Chem. Phys.*, **2005**, 144104.

[3] J. Hill, *Chem. Phys. Phys. Chem.*, **2006,** 4072-4078.

NANOCOMPOSITE POLYMER SENSOR MATERIALS FOR DETECTION OF HEAVY METAL ION CONTAMINANTS IN WASTE WATER

O. Zinchenko, V. Ezhova, O. Slisenko, A. Tolstov
Institute of Macromolecular Chemistry NASU, 48 Kharkivske shose, 02160 Kyiv, Ukraine
e-mail: a.tolstov@ukr.net

A versatile method of preparation of novel nanocomposite sensor materials based on hybrid hydrophilic acrylic matrix with chemically joined ZnO nanoparticles was proposed. Previously synthesized dispersion of modified ZnO nanoparticles (20 ± 4.5 nm) was obtained and introduced into a mixture of UV polymerizable acrylic acid (AA) / 2-hydroxyethyl methacrylate (HEMA) monomer mixture followed by curing under appropriate conditions.

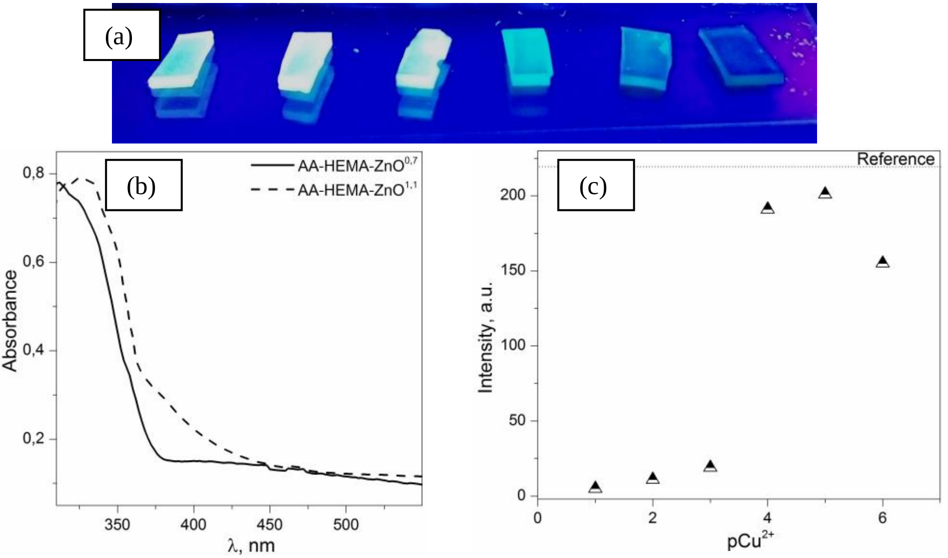


Fig. 1. Visualization of fluorescent properties (a), UV-vis absorbance curves (b) and intensity of fluorescence at different Cu^{2+} content (c) of the nanocomposites obtained

Structure and thermal characteristics as well as absoirbance and fluorescence parameters of hybrid poly(AA-co-HEMA)-g-ZnO nanocomposites obtained were characterized in details. The thin film nanomaterials demonstrate high heavy metal ions sensitivity under swelling conditions. A presence of Cu^{2+} ions at ultra-low concentration (as low as 10^{-6} M) substantially suppresses fluorescence of optically active ZnO nanoparticles of the hybrid nanocomposites. Moreover, the nanomaterials have high pH-responsive ability as well and could be used for elaboration of novel sensor materials with multiple sensing mechanisms for many applications.

THE BACTERICIDAL MATERIAL POLYURETHANE FOAM-I_2 BASED ON THE SORPTION OF IODINE FROM AQUEOUS AND ORGANIC SOLUTIONS

A. Yu. Trokhimenko
Taras Shevchenko Natiomal University, Volodymyrska, 64, Kyiv 01601, Ukraine
e-mail: annatrohimenko@ukr.net

The sorption and diffusion of small molecules in polymers is important in many areas of polymer technology such as packaging of foods, drugs, and cosmetics, controlled release of dissolved materials, treatment of waste waters, chromatographic analysis, and separation of gases. Iodine, povidone-iodine has been used as a multivalent, local, broad-spectrum antiseptic having bactericidal, fungicidal, sporicidal, protocidal, and virucidal properties.

Iodine sorption by polyurethane foams was studied using iodine water and organic solutions with hexanes, toluene, CCl_4 and $CHCl_3$. In the solution process, the equilibrium absorption followed the distribution law and the distribution coefficients varied depending on the solvent used.

Two different polyurethane foams used. All the foams were white, skin-free, and had an open-cell structure. The foam sample was cut to a size of 1,0x1,0x0,5 cm and extracted with acetone before use.

Iodine solutions with different concentrations were prepared in water and organic solutions. Each foam sample was immersed in a 50 mL iodine solution of fixed concentration for ca. 2 h to swell the foam and allow iodine to diffuse into the foam. The sample was then removed from the solution and squeezed to remove the solvent. The resultant foam was dried for ca. 1 h to evaporate any remaining solvent and then weighed (figure 1, 2).

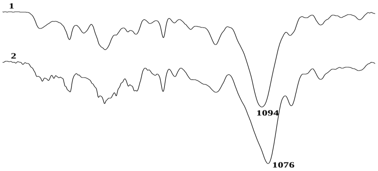


Figure 1. IR-spectra of Polyurethane foam (upper curve) and Polyurethane foam-I_2 (bottom curve)

Figure 2. The bactericidal material Polyurethane foam-I_2

The absorption equilibrium was achieved in a short time because of the ability of solvents to swell the polyurethane foams, and a uniform distribution of iodine in the polymer matrix was obtained. The equilibrium absorption in the polyurethane foams followed a distribution law and the distribution coefficients varied depending on the affinity of the solvent for iodine. Both aspects greatly depend on the interactions between polymers, iodine and solvents.

STRUCTURE AND MORPHOLOGY OF CRYPTOMELANE SAMPLES SYNTHESIZED BY DIFFERENT METHODS AND THEIR ACTIVITY IN THE REACTION OF SULFUR DIOXIDE OXIDATION WITH AIR OXYGEN

T.L. Rakitskaya, A.S. Truba, A.P. Nazar, T.A. Kiose, V.Y. Volkova
Faculty of Chemistry and Pharmacy, Odessa I.I. Mechnikov National University.
St. Dvoryanskaya 2, 65082, Odessa, Ukraine
e-mail: tlr@onu.edu.ua

Polymorphous manganese dioxide forms including cryptomelane (OMS-2) are more active than some other metal oxides in the reaction with sulfur dioxide. The cryptomelane samples were synthesized by potassium permanganate reduction with manganese sulfate (reflux method), OMS-2(Refl-3) and OMS-2(Refl-4), and also by KNO_3 and $MnSO_4$ melting together, OMS-2(MS). All the samples thus obtained were characterized by XRD method, SEM, and FT-IR spectroscopy. The cryptomelane samples (0.5 g each) were tested at 20 °C, an initial SO_2 concentration in the gas air mixture (GAM) of 150 mg/m^3, and a GAM volume flow rate of 16.6 cm^3/s. Data presented in Table show that only OMS-2(Refl-3) obtained in three steps during 24 hours contains bixbyite (Mn_2O_3) as an impurity phase. Sizes of cryptomelane crystallites are in the range from 11 to 15 nm.

Sample	Before reaction with SO_2		After reaction with SO_2		$Q_{sp}\cdot10^3$, mol SO_2/g	τ_{MPC}, min
	Phase (content, %)	D, nm	Phase (content, %)	D, nm		
OMS-2 (Refl-3)	$K_xMn_8O_{16}$ (90.5) Mn_2O_3 (9.49)	15 66	$K_xMn_8O_{16}$ (67.9) $MnSO_4\cdot H_2O$ (31.6)	10 38	1.64	120
OMS-2 (Refl-4)	$K_xMn_8O_{16}$ (100.0)	11	$K_xMn_8O_{16}$ (56.6) $MnSO_4\cdot H_2O$ (41.4)	10 59	3.56	390
OMS-2 (MS)	$K_xMn_8O_{16}$ (100.0)	14	$K_xMn_8O_{16}$ (57.9) $KMn(HSO_4)_2\cdot 2H_2O$ (4.5) $MnSO_4\cdot H_2O$ (37.6)	9 - 60	3.06	310

The activity of cryptomelane in the reaction with sulfur dioxide was characterized by the following parameters: τ_{MPC} is a period of time during which outlet SO_2 concentrations are lower than the maximum permissible concentration of sulphur dioxide equal to 10 mg/m^3, and Q_{sp} is a specific amount of SO_2 entered into the reaction to the moment when the outlet SO_2 concentration becomes equal to the inlet SO_2 concentration (150 mg/m^3). As can be seen, OMS-2(Refl-4) obtained in four steps during 24 hours is the most active sample. XRD, SEM, and FTIR spectroscopic data show that cryptomelane interaction with SO_2 is accompanied by formation of a new phase, $MnSO_4\cdot H_2O$, and also by a decrease in cryptomelane phase content and its crystallite size.

SOLIDPHASE EQUILIBRIA IN THE GeTe-Bi_2Te_3 SYSTEM AND CRYSTAL STRUCTURES OF THE INTERMEDIATE PHASES

[a]Alakbarova T.M., [b]Orijlu E.N., [b]Imamaliyeva S.Z., [b]Babanly M.B.
[a]*Baku State University, 23, Z.Khalilov, AZ-1148, Azerbaijan*
[b]*Institute of Catalysis and Inorganic Chemistry, ANAS, 113, H.Javid, AZ-1143, Azerbaijan*
e-mail: babanlymb@gmail.com

The complex tellurides formed in the A^{IV}-B^{V}-Te systems (A^{IV}-Ge, Sn, Pn; B^{V}-Sb, Bi) with the tetradimite-like layered structure are promising functional materials with thermoelectric and topological insulators properties [1-3].

This work presents the results of studies of solid-phase equilibria in the GeTe-Bi_2Te_3 system by DTA, XRD, and SEM methods.

Alloys of the system, each weighing 0.3 g, were obtained from previously synthesized and identified initial binary compounds according to the following procedure. The stoichiometric amounts of the starting compounds were fused in an evacuated quartz ampoule to 750^0C. Then the samples were quenched in cold water, followed by annealing for 800-1000 h at 450^0C. In addition, a series of alloys with compositions 75-100 mol% GeTe was also annealed at 570^0C.

The results of DTA, XRD, and SEM showed the formation in the system of 2 series of ternary compounds belonging to the homologous series $mBi_2Te_3{\cdot}nGeBi_2Te_4$ and $GeBi_2Te_4{\cdot}nGeTe$. Representatives of the first series are mixed-layer Van der Waals compounds with different alternations of 7 and 5 layer packets. Representatives of the second series are also Van der Waals compounds in which GeTe bilayers are introduced into seven-layered $GeBi_2Te_4$ and form packages consisting of 9,11,13, etc. layers. In the composition range> 90 mol% GeTe, the alloys annealed at 450^0C are solid solutions based on the low-temperature rhombic modification of GeTe, and the alloys annealed at 570^0C are solid solutions based on the high-temperature cubic modification of GeTe.

Based on the powder XRD, the types and parameters of the crystal lattices of the detected ternary compounds and solid solutions were determined

The work has been carried out within the framework of the international joint research laboratory "Advanced Materials for Spintronics and Quantum Computing" (AMSQC) established between Institute of Catalysis and Inorganic Chemistry of ANAS (Azerbaijan) and Donostia International Physics Center (Basque Country, Spain) and partially funded by a grant EİF/MQM/Elm-Tehsil-1-2016-1(26)-71/01/4-M-33.

[1] A.V.Shevel'kov, *Russ. Chem. Rev*, **2008, 77**, 1-19.
[2] M.B.Babanly, E.V.Chulkov, Z.S.Aliev et al., *Russ. J. Inorg. Chem.* **2017**, 62(13), 1703–1729
[3] K.Okamoto, K.Kuroda, Z.S.Aliyev et al. ,*Phys.Rev.B.*, **2012**, 86, 195304-195308

TEMPERATURE-TRIGGERED AGGREGATION OF PNIPAM-BASED CORE/SHELL NANOPARTICLES

L.O. Vretik[a], O.M. Chepurna[b], A.I. Marynin[c], O.A. Nikolaeva[a], T.Y. Ohulchanskyy[b]

[a] *Taras Shevchenko National University of Kyiv, Volodymyrs'ka Str., 64/13, Kyiv-01601, Ukraine*
e-mail: lvretik@gmail.com
[b] *College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, Guangdong, 518060, People's Republic of China*
[c] *National University of Food Technologies, Volodymyrska Str. 68, Kyiv, Ukraine*

Multifunctional nanoparticles (NPs) are extensively applied as drug delivery and cancer imaging agents [1]. Core-shell structure of polymer-based NPs provides possibility for feasible modification of their functional properties [2]. In our previous work, core-shell NPs were developed with core of polystyrene (PS) and poly(N-isopropylacryl amide) (PNIPAM) based shell. Such a design allowed us to load NPs with near infrared fluorescent dye and/or photosensitizer for fluorescence imaging in near and short-wave infrared spectral regions and imaging guided photodynamic therapy of cancer [3, 4].

PNIPAM-based NPs are known to exhibit temperature-dependent swelling-shrinkage behavior, similarly to bulk PNIPAM polymer [2]. The swelling-shrinkage temperatures for PNIPAM lay in physiological range that facilitates use of PNIPAM-based formulations in biomedical applications. In general, PNIPAM-based formulations used in biomedical field are obtained in a form of balk hydrogels or nanosized gels; in the latter case, aggregation of NPs is normally avoided to allow for intravenous administration [5].

Herein, we present a study of a temperature-triggered aggregation of shrunken polymer core-shell NPs. The core-shells NPs were synthesized and the inherent lower critical solution temperature (LCST) of PNIPAM-based shell (~32^{o}C) was tuned by copolymerization of NIPAM with hydrophilic monomers (e.g., acrylamide (AAm) or substituted acrylamide) to ~38-39^{o}C. The temperature-dependent behavior of core-shell NPs with different shells was investigated using dynamic light scattering (DLS) technique in broad temperature range and in different media; parameters of NPs aggregation were determined.

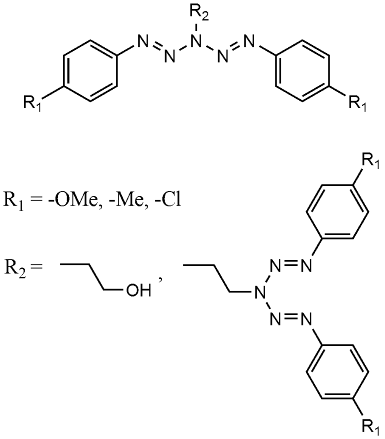
[1] M. Molina, S. Wedepohl, M. Calderon Polymeric near-infrared absorbing dendritic nanogels for efficient in vivo photothermal cancer therapy, *Nanoscale*, **2016,** 8, 5852–5856.
[2] M. Ballauff, Y. Lu, *Polymer*, **2007**, 48, 1815-1823.
[3] A. Yakovliev, R. Ziniuk , D. Wang et al, *Nanoscale Research Letters*, **2019**, 14(1), 243-254.
[4] O.M. Chepurna, A.Yakovliev, R. Ziniuk et al, *Journal of Nanobiotechnology*, **2020**, 18, 19.
[5] N. Vanparijs, L. Nuhn, B.G. De Geest *Chem. Soc. Rev.*, **2017**, 46, 1193-1239.

KINETICS OF FREE RADICAL POLYMERIZATION OF METHYL METHACRYLATE INITIATED BY PENTAZADIENES

Vyshnevsky D., Syromiatnikov V., Kolendo A.
Taras Shevchenko National University of Kyiv, 62a Volodymyrska St., 01601 Kyiv, Ukraine
e-mail: vyshnevsky@protonmail.com

The primary goal of synthetic polymer chemistry is to prepare polymers with controlled molecular weight and predefined architecture. Free radical polymerization is the most important industrial process to prepare high molecular weight polymers. Methyl methacrylate (MMA) is a key building block for acrylic based polymers. Kinetics of its free radical polymerization in different phases is well studied with presence of "classic" azo- or peroxide initiators. Using of polyaza compounds in free radical polymerization processes remains insufficiently explored. Decomposition of pentazadiene molecules like other linear unsaturated polyaza compounds is known to yield radicals of different structure and reactivity. Hence, polymerization of MMA will have a multistep character [1].

Kinetics of MMA thermal polymerization in DMF solution initiated by pentazadienes of different structure (Fig. 1) was studied by dilatometric method. Molecular weights of obtained polymers were established by GPC method. The correlations between rate of polymerization, molecular weight and initiator structure were found.



R$_1$ = -OMe, -Me, -Cl

R$_2$ =

Fig.1 Pentazadiene initiators structure

[1] V.Syromiatnikov et al, Chemical Engineering of Polymers, **2018**, 41-49

ORGANO-MINERAL COMPOSITE POLY(4 –VINYLPYRIDINE–*b*-STYRENE)-SILICA GEL: SYNTHESIS AND SORPTION PROPERTIES

M. Tovstenko-Zabelin[a], E.S. Yanovska[a], O. Kondratenko[c], O.A. Nikolaeva[a], D. Sternik[b], I.O. Savchenko[a], L.O. Vretik[a]
[a] *Taras Shevchenko National University of Kyiv, Volodymyrs’ka Str., 64/13, Kyiv-01601, Ukraine*
e-mail: lvretik@gmail.com; elina_yanovska@ukr.net
[b]*Maria Curie-Skłodowska University, 2 Maria Curie-Sklodowska Sq., 20-031 Lublin, Poland*
[c]*Ivan Franko Zhytomyr State University, 42 Pushkina Str., 10008 Zhytomyr, Ukraine*

Organic composite materials consisting of the water-insoluble polymer and mineral carrier with high sorption activity are promising adsorbents for the removal of toxic metal ions in waste water. To increase the sorption capacity of adsorbents, adsorption or chemical attachment to inorganic surfaces of N,O-containing polymers with complexing and ion-exchange properties is thus increasingly used. Semultaneous presense in the composite of N,O and S-atoms would higly increase its adsorption activity towards different types of metal ions.

In [1-3], we described the *in situ* immobilization of 4-vinylpyridine and styrene statistical copolymers on mineral carriers, e.g. silica gel and saponite clay. Obtained organo-mineral composites showed high sorption capacity to Pb (II), Cd (II), Zn (II), Cu (II), and Fe (III) ions.

This work is devoted to the syntheses of block-copolymers of 4-vinylpyridine and styrene with feed molar ratio 4:1 by RAFT polymerization. RAFT-mediated polymerization gave an opportunity to incorporate in each polymer chain an additional -S-C(S)- active moiety. Further aminolysis with hexylamine provided each polymer chain with –SH end-group.

The obtained S-functionalized block-copolymers were immobilized on the silica gel mineral carriers from the THF solutions. The amount of immobilized copolymer was calculated by thermogravimetry. The sorption properties of the obtained organo-mineral composites towards Pb (II), Cu (II), Fe (III) ions will be discussed.

[1] E.S. Yanovska, L.O. Vretik,, O.A. Nikolaeva et al, *Nanoscale Research Letters*., **2017**, 12, 217-222.

[2] E. S. Yanovska, L.O. Vretik, O. Kondratenko, O.A. Nikolaeva, D. Sternik and O. Yu. Kichkiruk, *Molecular Crystals and Liquid Crystals*., **2018**, 672(1, part 3), 104-114.

[3] E.S. Yanovska, O.A. Nikolaeva, O.U. Kondratenko, L.O. Vretik, French-Ukrainian Journal of Chemistry., **2019**, 7(2),145-152.

COMPOSITION AND MOLECULAR WEIGHT DISTRIBUTION OF SUBSTANCES FROM NATURAL COFFEE EXTRACTS

Kurta S. A., Khatsevich O.M., Yakubiak M.R.,
Chemistry Department, Vasyl Stefanyk Precarpathian National Universyty, Halytska str., 201/320 Ivano-Frankivsk, Ukraine. *E-mail:* kca2014@ukr.net ;

Research on the selection and analysis of odorous substances from natural products, such as different varieties of coffee was described. Parameters and equipment of process distillation with water vapor are given here for selection of coffee fragrances from specially prepared roasted, ground and extracted varieties of coffee, such as Arabica and Robusta. A literary patent review on the properties, preparation and its peculiarities for coffee of different varieties was carried out.

The aim of the work is to find alternative methods of roasting, grinding coffee beans and extracting coffee aromas and flavors, and studying the nanostructural properties of aqueous and alcoholic extracts of coffee of various varieties. In addition, the influence of coffee aroma and taste extracts on the metabolism of alcohol in the human body was investigated [1].

As a result of the research on isothermal roasting of green coffee grains of Arabica Brasil Santos and Robusta Vietnam, optimal technological conditions for roasting in a Microwave Isothermal Chamber "Disvery DY110" were installed in a glass flask with a magnetic stirrer (n = 150-250 rpm; time of roasting = 10-20 minutes, weight loss of coffee beans after roasting = 15-18%, roasting temperature from 145 - 195 ºC, power of microwave oven N = 300-900 Watts.

The technique of distillation of odorous and aromatic substances of coffee beans of milled coffee with water vapor and ethyl alcohol of various concentrations is improved. For the obtained water-alcohol aqueous extracts of coffee it was established that the hydrogen index of alcoholic extracts is approaching neutral values of pH = 4-6, which distinguishes them from acidic aqueous coffee extracts pH = 3-4, regardless of the grade of coffee. [2].

In the infrared spectra of coffee extracts the presence of caffeine and other fragrant substances of acid, ketone or aldehydes composition is observed. When analyzing the particle size of macromolecules of fragrant substances by static and dynamic molecular mass distribution of nanoparticles in size with a corner section of laser light (NANODS CILAS) in aqueous and alcoholic extracts, it is shown that their size in water extracts is an order of magnitude larger (90-9000 nm). While for coffee extracts in ethyl alcohol, these sizes are much smaller (150-1200 nm). Obviously this is the main cause of different aroma of coffee in water and in alcohol solution [2].

Alcoteter Alcofor-105 conducted a preliminary analysis of the metabolism of ethyl alcohol in the human body, depending on the concentration and volume of alcohol. . In this case, the catalytic effect of water-alcohol extracts of natural coffee on the metabolism and conversion of alcohol and acetaldehyde in the human body, which is 1.5-2.5 times faster than for ordinary solutions of alcohol in water, is recorded. Thus, for 1 hour when using ethyl alcohol of different volumes with extracted nanostructured substances of coffee aromas in water in exhaled air, it is possible to reduce the concentration of alcohol and acetaldehyde to 0.18% per milliliter - the permissible norm for drivers.

1 .Sergiy Kurta ., Olga Khatsevich ., Mariia Yakubiak. Nanostrukturalne właściwości ekstraktów substancji aromatycznych naturalnej kawy // Abstracty. IV Ogólnopolska Konferencja Naukowa Nanotechnologia wobec oczekiwań XXI w. Lublin, 13 grudnia 2019 r. Wydawnictwa Naukowego TYGIEL (www.bc.wydawnictwo-tygiel.pl)., Poland. p.19.

ADSORPTION PROPERTIES OF NATURAL ALUMOSILICATE UKRAINIAN MINERALS, *IN SITU* MODIFIED BY POLY [8-METHACROYLOXYQUINOLINE] TO Pb(II), Mn(II), Cu(II) AND Fe(III) IONS

I. Savchenko[1], E. Yanovska[1], D. Sternik[2], O. Kychkyruk[3]
[1]Taras Shevchenko National University of Kyiv,
60, Volodymyrska str., 01601 Kyiv, Ukraine
[2]Maria Curie-Skłodowska University,
Maria Curie-Sklodowska Sq., 20-031 Lublin, Poland
[3]Ivan Franko Zhytomyr State University,
42 Pushkina Str., 10008 Zhytomyr, Ukraine
e-mail: elina_yanovska@urk.net

Nature has created safe methods of water purification, which are the adsorption of anthropogenic pollutants during the passage of water through the horizons of minerals (clays, silicates and aluminosilicates, zeolites, etc.) and allow to preserve its structure and mineralization. This mechanism worked and maintained equilibrium between the planet's geo spheres throughout their existence. Accordingly, its reasonable use should be the basis of water and wastewater treatment technologies that can be converted into soluble form. The use of such natural minerals of Ukraine as Podolsky saponite (saponite clay), Transcarpathian clinoptilolites of Sokirnytsia and Tushin deposits, bentonite, vermiculite, colored clays of Lugansk region and Crimea are promising as ecologically safe industrial adsorbents-purifiers. They are known for their good adsorption properties, and therapeutic and healing properties.

It is advisable to use composite materials based on natural minerals extracted in Ukraine to solve specific environmental problems, namely for industrial wastewater treatment,. We have shown earlier that *in situ* immobilization of the surface of Podilsky saponite and Sokyrynitsky clinoptilolite with polyaniline leads to an increase in the sorption capacity of these minerals with respect to phosphate and arsenate ions in a neutral aqueous medium 2-3 times. *In situ* immobilization of the surface of the Tashkiv field saponite and the Tushin field clinoptilolite by complexing polymers, such as poly [N- (4-carboxyphenyl) methacrylamide] or poly [4-methoxyloxy- (4'-carboxy-2'-nitro) azobenzene] increases their sorption capacity in neutral aqueous medium with respect to Pb (II), Cd (II), Cu (II) and Fe (III) ions.

This work is devoted to the *in situ* immobilization of poly [8-methacroyloxyquinoline] on the surface of saponite of Tashkiv field, clinoptilolite of Tushin field and vermiculite and adsorption properties of the synthesized composite material on ions Pb(II), Mn(II), Cu(II) та Fe(III). The fact of polymer immobilization is confirmed by IR spectroscopy. The amount of immobilized polymer in the composition of the synthesized material is established according to thermogravimetric analysis. Using scanning electron microscopy, the surface morphology of the modified silica gel was established. It has been found that the best adsorption properties for all selected metal ions among the synthesized composites are modified clinoptilolite.

FLUORESCENT TECHNIQUES FOR REGISTRATION OF DRUG REDISTRIBUTION FROM NANOSIZED CARRIERS

V. Zorin[1,2], T. Zorina[1], I. Kravchenko[1], N. Kutsevol[3]
[1]*Belarussian State University, pr. Nezavisimosti 4, Minsk, 220030 Belarus.*
E-mail: zorinat@bsu.by
[2]*International State Ecological Unversity named after A.D.Sakharov BSU, Dolgobrodskaya Street, 23/1, Minsk, 220070, Republic of Belarus*
[3]*Faculty of Chemistry, Taras Shevchenko National University of Kyiv, 60*

Volodymyrs'ka str., 01601 Kyiv, Ukraine

The majority of 2nd generation photosensitizers are nonpolar tetrapyrrolic compounds with poor water-solubility, thus requiring special drug formulations of liposomes, polymers, oil emulsions and solvent mixtures for their injection. Incorporation into such structures provides a stable monomeric state of photosensitizer. Additional advantages of applying carriers are associated with the possibility of using the features of biodistrubition processes of nanocarriers (passive targeting, phagocyte binding specificity, etc) to control the photosensitizer pharmacokinetics. This work is related to the search for methods for controlling the processes of photosensitizer release from nanocarriers in biological systems

Several approaches to the analysis of the rate of chlorin-type photosensitizers release from unilamellar lipid vesicles and stimul-dependent polymer nanocarriers in model biological systems are studied: spectroscopic parameters, the excitation energy transfer from fluorescent probe diphenylhexatrien to meta-tetra(hydroxyphenyl)chlorin (mTHPC), measurements of mTHPC fluorescence anisotropy and photoinduced mTHPC fluorescence quenching. Each approach possesses characteristic range of sensitivity to local mTHPC concentration. The use of fluorescence anisotropy allows for quantitative estimation of redistributed mTHPC in the range of mTHPC:lipid ratios of 1:100-1:1000, the excitation energy transfer from diphenylhexatrien to mTHPC is sensitive upon the ratios of less than 1:200, and photoinduced quenching – 1:10-1:500. According to the data obtained the fluorescent spectroscopic characteristics are the most reliable and informative parameters for controlling photosensitizers release and redistribution from nanocarriers. We provide various examples of applying the proposed techniques for study of kinetic behavior of photosensitizers loaded into nanocarriers.

This publication is supported in part by the Ministry of the Education and Science of Ukraine: joint Ukrainian-Belarusian research and development projects M110-2019 (2019-2020) and with the financial support of the Belarusian Republican Foundation for basic research, grant no. M19UKRG-002.

SECTION 7

NANOCOMPOSITES AND LASERS IN MEDICINE AND BIOLOGY

MORPHOLOGICAL AND PROPERTIES CHARACTERIZATION OF NOVEL BIOCOMPOSITES OF POLY(3-HYDROXYBUTYRATE-CO-3-HYDROXYHEXANOATE) (PHBHHx)/ALOE VERA FIBERS

Mustapha Kaci[a], Nadjet Dehouche[a], Celia Idres[a], Idris Zembouai[a], Stéphane Bruzaud[b]
[a] *Laboratoire des Matériaux Polymères Avancés (LMPA), Université de Bejaia 06000, Algeria*
[b] *Institut de Recherche Dupuy de Lôme (IRDL), Université de Bretagne-Sud, Rue Saint Maudé, 56321 Lorient Cedex, France*
e-mail: kacimu@yahoo.fr

In recent years, biodegradable polymers and natural fibers are gaining growing interest towards developing environmentally friendly materials as an alternative to petroleum based products [1]. Thus, new developments in the field of renewable and biodegradable polymers are being intensified. In this context, PHBHHx, which is a random copolymer of 3-hydroxybutyrate and 3-hydroxyhexanoate, is fully biodegradable polyesters belonging to the polyhydroxyalcanoates (PHA) family. PHBHHx is produced by the fermentation of bacteria or other microorganisms as intracellular reserve of carbon or energy. Due to its ductile nature and wider processing window compared to poly(3-hydroxybutyrate), PHBHHx is used in a broad range of applications in various industries such as biomedical sector [2]. Among the biodegradable reinforcements, a new kind of natural cellulosic fibers is extracted from the leaves of Aloe Vera Cactus plant, which is a member of the Agavoideae family [3]. This plant is largely available in Algeria and it is used in cosmetic and pharmaceutical industry and more recently in textile industry in India [4]. However, the effectiveness of natural fibers as reinforcement can be improved by enhancing the interfacial adhesion between the fiber and the polymer matrix through various fiber surface treatments.

In this paper, novel biocomposites based on PHBHHx and alkaline treated Aloe vera fibers (AVF) incorporated at 20 wt%, were prepared by melt compounding. The effect of the fiber surface treatment on morphology and physical properties of the PHBHHx biocomposite was investigated and the results discussed in relation to those obtained before treatment. Scanning electron microscopic analysis (SEM) showed that the alkaline treatment of AVF was essential to eliminate the formation of aggregates in the PHBHHx matrix and to ensure a better interfacial adhesion between the natural fibers and the polymer. The treated PHBHHx biocomposite exhibited increased rheological properties compared to untreated one.

[1] C. A. Murphy, M.N. Collins, *Polym. Comp.*, **2016**, 39, 1–10.
[2] N. Dehouche, I. Celia, M. Kaci, I. Zembouai, S. Bruzaud, *Polym.Degrad. Stab.*, **2020**, 175, 109131 (1-10).
[3] A. N. Balaji, K. J. Nagarajan, *Carbohydr. Polym.*, **2017**, 174, 200–208.
[4] S. Chaitanya, I. Singh, *Int. J. Precis. Eng. Manuf. - Green Technol.*, **2018**, 5, 143–150.

AGGREGATIVE STABILITY OF RARE-EARTH BASED NANOPARTICLES IN DIFFERENT MICROENVIRONMENTS AND BIOLOGICAL MEDIA

Katherine Averchenko, Nataliya Kavok, Ganna Grygorova, Vladimir Klochkov
Institute for Scintillation Materials NAS of Ukraine, 60 Nauky ave., 61072, Kharkiv, Ukraine
e-mail: *katherine.averchenko@gmail.com*

Nanoparticles (NPs) have found wide range of applications owing to their physicochemical and redox properties. The stabilization of NPs against aggregation in high-ionic-strength solutions such as biological media is one of the most important problems for their biomedical application.

In present work we have estimated the aggregative stability of rare-earth based NPs ($LnVO_4$:Eu^{3+} (Ln = Gd, Y, La) and CeO_2 with different form-factors and sizes) in different biological media. Also the influences of separate protein (or their mixture) – bovine serum albumin (BSA), immunoglobuline G, holo-transferrin, fetal bovine serum (FBS) as well as relevant media compounds as glutathione, on the aggregative stability of NPs were investigated.

Aggregative stability of NPs was studied using dynamic light scattering techniques in biologically relevant solutions and media: 5% glucose, 50 mM Tris buffer (with different pH within of physiological values), Igla MEM medium, Krebs-Ringer buffer, HBSS-buffer, in the absence or presence of the proteins, for 30 minutes and 24 hours. The effect of oxidized and reduced glutathione on the stability of NPs in Tris buffer at various physiological pH (range 6.7, 7.4, 7.8) was also determined.

The aggregation of NPs was observed in saline systems. The highest degree of aggregation was observed for Igla MEM and Krebs-Ringer buffer, while extra small NPs (2 nm) exhibited the highest aggregative instability. In contrast, no changes in diameter of NPs have been observed in 5% glucose solution. Tris or Hepes organic buffers show lower destabilization influences as compared to Igla MEM and Krebs-Ringer buffer. In all media, albumin (0.2%) prevents aggregation of NPs. Albumin also stabilizes NPs in buffer and water glutathione solutions regardless of pH. Immunoglobulin induces the hydrodynamic diameter increase, but not in the composition of protein mixture (main serum proteins in their proper ratio). Starting from 1-2% FBS prevent NPs aggregation that can be explained by multilayer protein corona formation.

Obtained results suggest that in contrast to organic buffer and 5% glucose, any relevant biological media or salt-containing buffers induce the NPs aggregation. The role of albumin in optimizing the conditions for biological applications of NPs was revealed. Physico-chemical properties of NPs affect the dynamics of formation and composition of the protective protein crown.

KEY WORDS: rare-earth based nanoparticles, aggregation stability, protein crown.

EFFECT OF DIFFERENT DOSES OF SILVER NANOPARTICLES IN POLYMER MATRIX TREATMENT ON FEMALE REPRODUCTIVE FUNCTION IN MICE

Sribna Valentyna[1], Kaleinikova Oksana[1], Kuziv Yulia[2], Lytvynenko Alina[1], Vinogradova-Anyk Olena[3], Karvatskiy Igor[3], Voznesenskaya Tetiana[1], Blashkiv Orest[3], Kutsevol Natalia[2]
[1] *Bogomoletz Institute of Physiology, NAS of Ukraine, Kyiv, Ukraine*
[2] *Taras Shevchenko National University of Kyiv, Kyiv, Ukraine*
[3] *Bogomoletz National Medical University, Kyiv, Ukraine*
e-mail: tblashkiv@gmail.com

Recently, it has been proved that copolymers with dextran cores and grafted polyacrylamide are effective in photodynamic and chemotherapy [1], as well as, silver nanoparticles with their unique optical, electron and antibacterial properties are already widely used in biosensors, photonics, electronics as antimicrobial and antitumor [2]. However, further research is needed to define correct dosage and to assess the risks. Thus, animal studies are becoming more relevant to determine the effect of the treatment of such drug nanosystems on female reproductive function in particular.

This study aims to evaluate the effect of a one-time treatment of different doses of polymer matrix (D-PAA) and silver nanoparticles in polymer matrix (AgNPs-D-PAA) on reproductive function.

The star-like polymer matrixes D-PAA were loaded with silver nanoparticles. The size of such silver nanoparticles is 8-15 nm. A technique for estimation of pre- and post-implantation death rates, *in vitro* meotic maturation of oocytes, double fluorescent vital assay and statistical analysis were used.

No significant changes in the number of oocytes isolated from one ovary and meiotic maturation of such ovarian oocytes *in vitro*, the number of living cells of follicular environment of oocytes and the number of such cells with morphological signs of apoptosis and necrosis, pre- and post-implantation mortality rates of embryos and the number of live newborns have been established under conditions of one-time treatment with dextran-polyacrylamide at doses of 0.39 mg/kg and 3.90 mg/kg and AgNPs-D-PAA at doses of 0.20 mg/kg and 2.0 mg/kg.

Thus, new data have been obtained and the effect of AgNPs-D-PAA and D-PAA on somatic and germ cells in mammals has been evaluated, which has not been previously done.

1.Kutsevol N., Naumenko A., Harahuts Yu. et al., New hybrid composites for photodynamic therapy: synthesis, characterization and biological study // Applied Nanoscience, 2019, 9:5:881-888. https://doi.org/10.1007/s13204-018-0768-y

2. Braun GB, Friman T, Pang HB, Pallaoro A, Hurtado de Mendoza T, Willmore AM, et al. Etchable plasmonic nanoparticle probes to image and quantify cellular internalization. Nat Mater 2014; 13(9): 904-911.

ECO-FRIENDLY SYNTHESIS OF Ag_2S NANOPARTICLES, THEIR OPTICAL AND ANTIMICROBIAL PROPERTIES

Mariya Borova[1], Antonina Naumenko[2], Olga Kapush[3], Svetlana Plokhovska,[1] Inna Horiunova[1], Alla Yemets[1]
[1]*Institute of Food Biotechnology and Genomics NAS of Ukraine, Osipovskogo st. 2a, Kyiv-04123, Ukraine. e-mail: marie0589@gmail.com*
[2]*Taras Shevchenko National University, Faculty of physics, Prospect acad. Glushkova, 4, Kyiv-03022, Ukraine.*
[3]*V.E. Lashkaryov Institute of Semiconductor Physics NAS of Ukraine, Pr. Nauki 45, Kyiv 02000*

Silver sulfide (Ag_2S) nanoparticles possess unique semiconducting, optical, and electrical properties and are highly stable. They are broadly used in solar cell batteries, thermoelectric sensors, biosensors [1]. An alternative approach to nanoparticle production under mild conditions can be a biotechnological process with biological matrices. Common requirements imposed on nanoparticles include reproducibility, narrow shape and size distribution, stability, a simple protocol, and the absence of toxic substances. The purpose of this study is to develop a new eco-friendly method for biosynthesis of Ag_2S nanoparticles by *Pleurotus ostreatus* and to estimate their antibacterial effects.

P. ostreatus was grown in 100 mL flask with 50 mL of Glucose Yeast Peptone liquid medium under 28˚C for 10 days. 0,025 M solutions of $AgNO_3$ and Na_2S were poured into the flasks with fungal mycelium in order to produce Ag_2S. Absorption spectra were measured using a spectrophotometer Specord UV-VIS. Luminescence spectrum were measured using a Cary Eclipse serial spectrophotometer (Varian Inc., Agilent Tech, USA). *Escherichia coli* and *Bacillus thurengensis* were used to study the antibacterial properties of Ag_2S nanoparticles at the following concentrations: 3, 1.5, 1, 0.6, 0.3 mg/mL. Paper discs were soaked with different concentrations of Ag_2S and placed on the surface of Petri dishes with bacterial strains. The incubation was carried out in a thermostat at a temperature of + 37 ° C for 24 hours. Measurement of lysis zones of *E. coli* and *B. thurengensis* was performed using a software Image J (1.38 d).

It was found that absorption maxima of Ag_2S nanoparticles corresponded to $\lambda_m \sim 315$ nm and 470 nm. Luminescent spectrum had a wide peak at 520 nm. Obtained nanoparticles have a spherical shape and a size within 20 – 25 nm. Tested strains of *E. coli* and *B. thurengensis* are sensitive to Ag_2S nanoparticles. Inhibition of bacterial growth was observed under high concentration of these nanoparticles (3 and 1.5 mg/mL). Thus, antibacterial effects of synthesized Ag_2S in combination with luminescent properties and nanosize allows them to be used as nontoxic labels or nanocarriers in cell biology applications.

[1] Sadovnikov S.I., Kuznetsova Y.V., Rempel A.A. Ag2S silver sulfide nanoparticles and colloidal solutions: Synthesis and properties. Nano-Structures & Nano-Objects., 2016, vol.7, p. 81–91.

INTERPLAY OF ANTIBIOTIC GRAMICIDIN S WITH CHOLESTEROL AND DEXTRAN-POLYACRYLAMIDE COPOLYMERS IN LIPID MEMBRANES

L.V. Budianska[a], V.P. Berest[b], N.V. Kutsevol[c], Y.I. Kuziv[c], O.V. Vashchenko[a]
[a] *Institute for Scintillation Materials of NASU, ave. Nauky, 60, Kharkiv, 61172, Country;*
[b] *V.N.Karazin Kharkiv National University, sqr. Svobody, 4, Kharkiv, 61022, Ukraine;*
[c] *Taras Shevchenko National University of Kyiv, str. Volodymyrska, 60, Kyiv, 01601, Ukraine*
e-mail: l.budjanskaja92@gmail.com

Gramicidin S (GS) is a widely used antibiotic since 1943. However, this effective membranoactive drug has heavy side effects, *viz.*, hemolytic one. It was established that GS interactions with lipid membranes is largely tuned by their lipid composition [1]. In particular, cholesterol (Chol) in high concentration hinders GS binding with lipid membranes [2], whereas in low concentration it promotes this process [1].

In the present work, gramicidin S (GS) was probed by means of differential scanning calorimetry (DSC) in model membranes of dipalmitlyphosphatidylcholine (DPPC) in concert with Chol or a negatively charged star-like dextran-polyacrylamid copolymer (D-g-PAA(PE)).

Specific membranotropic effect of GS, by the evidence of DSC, consisted in splitting of initial peak of DPPC membrane into two constituents, which reveal simultaneous binding of both GS monomers and GS olygomers. Critical Chol concentration in DPPC membrane was established which corresponds to qualitative changes of GS membranotropic effect. This finding accommodates differences in literature data concerning opposite Chol effects on GS binding with lipid membranes.

Joint introduction of GS and D-g-PAA(PE), which could be efficient nanocarrier for drug delivery [3, 4], into DPPC membrane allows one to trace certain modulation of GS effects in two aspects: (1) diminishing of total effect of GS; (2) favoring of GS olygomers binding with membrane.

The result points to a possible mechanism of minimization of negative side effects of GS.

[1] S. Afonin, e.a., *BBA. Biomembranes,* **2014**, 1838, 2260-2268.
[2] T. Abraham, e.a., *BBA. Biomembranes*, **2014**, 1838, 1420-1429.
[3] L. Li, K. M. Huh, *Biomater. Res*., **2014**, 18, 1-14.
[4] N. Kutsevol, e.a., *Mol. Cryst. Liq. Cryst.*, **2018**, 671, 9-16.

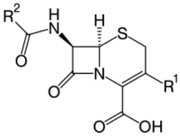
CHEMICALLY CROSS-LINKED HYBRID HYDROGELS FOR PROLONGED RELEASE OF ANTIBIOTICS

Oksana Nadtoka, Volodymyr Doroschuk, Serhii Lelyushok, Nataliya Kutsevol
Taras Shevchenko National University of Kyiv, 64/13, Volodymyrska Street, Kyiv 01601, Ukraine
e-mail: oksananadtoka@ukr.net

Hydrogels are three-dimensional cross-linked polymeric networks that can swell dramatically in an aqueous medium such as body fluids, while maintaining its structure and controlling drug release. Polymer networks have shown the promise as a way of incorporating antimicrobial agent into polymer such as the antibiotic streptomycin sulfate [1] or tetracycline [2] where the polymer networks act as a carrier for the antibiotics delivery system.

The polysaccharide Dextran not only are highly hydrophilic, biodegradable, but also more closely mimic the nature extracellular matrix glycosaminoglycans. Here, a chemically cross-linked hybrid hydrogels based on copolymer Dextran-graft-Polyacrylamide were synthesized by the radical polymerization in presence of difference amounts of cross-linking agent. Hence, hydrogels of varying cross-linking density were obtained.

Cephalosporins such as cefuroxime, cefazolin, ceftriaxone were used as model antibiotics for drug encapsulation and release behaviors studies:



Due to its high efficacy and low toxicity, cephalosporins rank among the first in clinical use. The mechanism of their action is related to the damage to the cell wall of bacteria in the reproductive stage, and the release of autolytic enzymes, which leads to their death. To understand the effect of the molecular transport of liquids into hydrogels on the drug release, swelling measurementwas carried out by immersing the hydrogels in physiological solution (pH 7.4) at 37°C. Obtained hydrogels possess good swelling capacity and diffusion rate. Cephalosporins release *in vitro* was determined using an UV spectrophotometer.

Finally, the antibacterial property of drug-loaded hydrogels was further explored. Antibiotic-loaded hydrogels were formed *in situ*, and could kill both Gram-positive bacteria and Gram-negative bacteria, indicating that the hydrogel as a wound dressing could provide protection against bacterial infection. Notably, the drug release was controlled via modifying the hydrogel structure. Therefore, the cross-linked hydrogels based on hybrid hydrogels as a promising carrier have potential application for wound healing.

[1] Song, A., Rane, A. A., & Christman, K. L. Antibacterial and cell-adhesivepolypeptide and poly(ethylene glycol) hydrogel as a potential scaffold for wound healing. Acta Biomaterialia, 2012, V. 8, pp. 41–50.

[2] Paul, W., Sharma, C. P. Chitosan and alginate wound dressings: A short review. Trends in Biomaterials and Artificial Organs, 2004, V. 18, pp. 18–23.

APPLICATION OF INTERNAL CAPACITANCE COMPENSATION OF REACTIVE POWER IN SINGLE-PHASE INDUCTION MOTORS

Zablodskiy M.M., Chuenko R.M.
National University of Life and Environmental Sciences of Ukraine
Heroyiv Oborony street 12, Kiyv, 03041, Ukraine
Email: Roman_chuenko@ukr.net

In addition to the disadvantages inherent for three-phase induction motors (the consumption of two types of power: active and reactive, high starting current, relatively low power factor), single-phase capacitor induction motors have their own. In particular, with single-phase power supply, these motors produce a pulsating magnetic field at zero starting torque. The efficiency and power factor of a single-phase induction motor are even lower than that of a three-phase one [1].

The purpose of the research is to increase the energy efficiency of single-phase capacitor induction motors by using internal capacitive compensation of reactive power [2].

Internal capacitive compensation of reactive power in asynchronous machines can be accomplished by combining the functions of the stator windings as working windings of the asynchronous machine and compensating by switching them on the circuit of the rotary autotransformer for electrical capacity. In this case we use the property of the autotransformer as the exchange of energy between the windings and the load (in this case, the capacitive load of the autotransformer) by electric and electromagnetic means also appears the magnetizing effect of the capacitive current in the ferromagnetic devices. The design of the stator of asynchronous machines allows choose an arbitrary angle of spatial shift between the windings axis of the rotary autotransformer.

For application of internal capacitive reactive power compensation, the stator winding of a single-phase induction motor is divided into two semi-windings having the same number of turns. These semi-windings have to be switched on by the circuit of the rotary autotransformer to the electric capacitance. The spatial displacement of the phase axes of the motor windings of the stator motor should be 90^{o} (for a three-phase motor it is advisable to choose the value of this angle 30^{o}). In this case, the number of phases doubles, resulting in the creation of a rotating magnetic field, which is no longer pulsating. As a result of the interaction of the rotating magnetic field of the stator with the winding of the rotor with a current, a greater than zero starting torque of the motor will be created. In this case it becomes possible to start a single-phase compensated induction motor at relatively low load (up to 0.5 from nominal).

The use of internal capacitive compensation of reactive power in a single-phase induction motor allows to increase its energy efficiency (the efficiency and power factor), as well as to improve its starting and adjusting characteristics.

[1] Vol'dek A.Y. Elektrycheskye mashyni / Vol'dek A.Y. – L.: Enerhyya, 1976 – 832.

[2] Mishyn V.I. Kompensovani asynkhronni mashiny: monohrafiya / Mishyn V.I., Makarevish S.S., Chuyenko R.M., Gavriluk V.V. – K.: Komprint, 2015. – 221.

THERMAL ASSISTED ANTI-STOKES LUMINESCENCE AND LASER COOLING EFFECT OF TRICARBOCYANINE DYES

O.P. Dimitriev[a], O.M. Fedoryak[a], I.P. Sharanov[b], Yu.L. Slominskii[b]
[a]*V.Lashkaryov Institute of Semiconductor Physics NAS of Ukraine, pr. Nauki 41, Kyiv 02028, Ukraine, e-mail: dimitr@isp.kiev.ua*
[b]*Institute of Organic Chemistry NAS of Ukraine, 5 Murmanska Str., Kyiv 02660, Ukraine*

Hot-band absorption (HBA) assisted anti-Stokes photoluminescence (ASPL) in the NIR region is demonstrated using novel tricarbocyanine dyes, with large anti-Stokes shifts up to 100 nm. Intensity of the ASPL is shown to correlate with intensity of the HBA through thermal population of ground-state vibronic levels (Fig.1). Molecular backbone bending leading to isomerization is found to be the dominant vibronic mode to assist in the above phenomenon. As a proof-of-principle, laser cooling effect for this type of molecules is demonstrated, with cooling power of ~1 mW per 100 mW of the pumping power, or cooling efficiency of 1% [1].

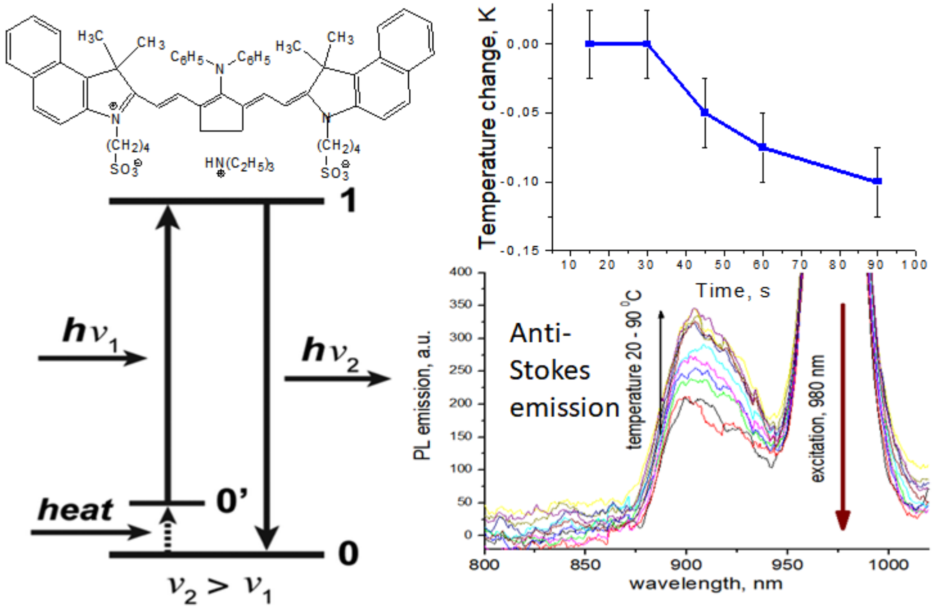


Fig.1. Dye structure, scheme of ASPL, ASPL spectra as a function of temperature and laser-cooling effect upon excitation of dye solution at 980 nm.

---

[1] O. Dimitriev, A. Fedoryak, Yu. Slominskii, A. Smirnova, T. Yoshida. *Chem. Phys. Lett.*, **2020**, 738, 136905.

HOST–GUEST COMPLEXES OF MEFENAMIC ACID AND β-CYCLODEXTRIN DERIVATIVES: SPECTROSCOPIC STUDY

G.V. Grygorova, V.K. Klochkov, S.L. Yefimova, Yu.V. Malyukin
Institute for Scintillation Materials NAS of Ukraine, 60 Nauky ave., 61072 Kharkiv, Ukraine
e-mail: grigorova@isma.kharkov.ua

Mefenamic acid (MA) is a potent nonsteroidal drug with strong analgesic, anti-inflammatory and anti-pyretic properties, widely applied in therapeutics [1,2]. It is highly prescribed in the treatment of rheumatoid arthritis, osteoarthritis, and other joint diseases. However, its oral bioavailability is very low, probably due to poor solubility in water and insufficient dissolution rate. Thus there is a need to find an approach to increase its oral bioavailability by enhancing its dissolubility using a pharmaceutical carrier. In recent years, inclusion complexes with cyclodextrin (CDs) have been widely used to improve the solubility of water-insoluble drugs, enhance the physical and chemical stability of drugs, eliminate undesired properties of drugs, and improve the bioavailability.

The inclusion complexation behavior, characterization and binding ability of MA with β-cyclodextrin and its derivatives were investigated in the solution state by means phase solubility studies and UV–vis spectroscopy. The results showed that the water solubility and stability of MA were obviously increased in the inclusion complex with CDs. The stoichiometry of the formed complexes were examined by means of the continuous variation method (the Job plot). Stability constants for the MA-CDs inclusion complexes have been calculated using the Benesi–Hildebrand method, while the thermodynamic parameters of reaction, i.e., the free energy change (ΔG), the enthalpy change (ΔH) and the entropy change (ΔS) have been estimated using the van't Hoff equation.

The solid MA-CDs complex was prepared by the co-evaporation method. The evidence for the host-guest solid complex formation was quantitatively estimated by differential scanning calorimetry (DSC) and Fourier transform infrared spectroscopy (FT-IR) analysis. Obtained results confirm energetically favorable interactions between MA and CDs molecules in solid state. This study presents new data, which could help in the development of pharmaceutical formulations with optimal drug release profile.

[1] S.M. Grant, S.P. Clissold Mefenamic acid: a review of its pharmacodynamic and pharmacokinetic properties, and therapeutic use in superficial and systemic mycoses, *Drugs*, **1989**; 37, 310-344.

[2] D Beule, K Van, V. Gestel Pharmacology of Mefenamic acid, *Drugs*, **2001**, 61 (Suppl. 1), 27-33.

CONTROLLED PRO/ANTIOXIDANT ACTIVITY OF $GdYVO_4:Eu^{3+}$ NANOPARTICLES

K.O. Hubenko, S.L. Yefimova, P.O. Maksimchuk, N.S. Kavok, V.K. Klochkov,
Yu.V. Malyukin
Institute for Scintillation Materials NAS of Ukraine, 60 Nauky Ave., Kharkiv 61072, Ukraine
e-mail: gubenko@isma.kharkov.ua

Nanoparticles (NPs), which promote generation of reactive oxygen species (ROS) and stimulate the onset of oxidative stress responsible for the development of a variety of adverse conditions, are of great prospect for various nanomedicine applications.

ROS generation in semiconducting NPs is a complex process, the efficiency of which is governed by both NPs characteristics (size, morphology, etc.) and external conditions, such as type of irradiation. It is well known that the irradiation of semiconducting NP with the light, which energy is greater than the NPs band gap, provokes the generation of holes (h^+) in the valence band and electrons (e^-) in the conduction band. The band structure of semiconductor NPs prevents the instantaneous recombination of free charge carriers. Thus, electrons and holes possess high reducing and oxidizing ability and can react with molecular oxygen and water molecules to produce different ROS.

On the other hand, in NPs characterized by high amount of structural defects, for instance, oxygen vacancies (VO) in oxide NPs, such defects could serve as traps for charge carriers and are responsible for ROS production in NPs even without UV irradiation (in the dark).

In our previous works, we have shown that $GdYVO_4:Eu^{3+}$ NPs exhibit photo-catalytic activity (ROS production) at both UV-light irradiation [1, 2] and in the dark condition [3].

In this work, we have studied light-triggered properties of $GdYVO_4:Eu^{3+}$ NPs in different biological environments including ascorbic acid, lipid suspensions and cell membranes. These studies have revealed that $GdYVO_4:Eu^{3+}$ NPs exhibit prooxidant activity at UV-light irradiation and antioxidant activity in the dark condition. Mechanisms will be discussed.

[1] Yefimova, S.L.; Maksimchuk, P.O.; Seminko, V.V.; Kavok, N.S.; Klochkov, V.K.; Hubenko, K.A.; Sorokin A.V., Kurilchenko, I.Yu.; Malyukin, Yu.V. *J. Phys. Chem. C.* **2019**, 123, 15323−15329.

[2] Hubenko, K.; Yefimova, S.; Tkacheva, T.; Maksimchuk, P.; Borovoy, I.; Klochkov, V.; Kavok, N.; Opolonin, O.; Malyukin, Yu. *Nanosc. Res. Lett*. **2018**, 13, 101–109.

[3] Pavel O. Maksimchuk, Svetlana L. Yefimova, Kateryna O. Hubenko, Valeriya V. Omelaeva, Nataliya S. Kavok, Vladimir K. Klochkov, Alexander V. Sorokin, Yuri V. Malyukin. *Phys. Chem. C.* **2020**, in press.

PHOTDYNAMIC THERAPY IN THE TREATMENT OF PATIENTS WITH NEUROPATHIC AND ISCHEMIC DIABETIC FOOT SYNDROME

Tetiana Kharchenko, Oksana Melekhovets, Yuriy Melekhovets, Alevtuna Radko
Sumy State University, Ministry of Education of Ukraine, Sumy
e-mail: kharchenko24t@gmail.com

Introduction. Diabetic foot syndrome (DFS) develops in 10% of patients with diabetes mellitus (DM). 50% of total diabetic cohort are at risk. Improving of prevention and treatment can reduce the amputation rate by 85%. Photodynamic therapy (PDT) is considered as a non-invasive procedure, safe and clinically approved, recognized as a promising therapeutic strategy to stimulate wounds healing.

The **aim** of the study is to evaluate the effectiveness of photodynamic therapy in the treatment of patients with neuropathic and ischemic diabetic foot syndrome.

Materials and methods. The study included 45 outpatients with type 2 DM with DFS II grade by Wagner, with an area ≤ 5 cm^2. At the baseline, all patients had wound bacteriological examination to prescribe appropriative antibiotics. Patients were divided into 2 groups depending on the ulcer etiology factor. Patients with ischemic ulcers were included in the 1st group (n = 22), patients with neurotrophic ulcers (n = 23) – in the 2nd group. Basic treatment included antibiotics and debridement of the wound (dressings with antiseptics, water-soluble ointments). Unloading of the lower limb was prescribed in the 2nd group; supervised exercise training - in the 1st group. PDT procedures were added to the basic therapy in both groups.

A laser machine “Lika-Surgeon M” (Photonica - Plus, Ukraine) with a wavelength of 660 nm were used for PDT. 10 procedures with continuous regiment were performed every other day. Methylene blue 1% aqueous solution was used as a photosensitizer.

The results of treatment were evaluated in 2 and 4 weeks with digital photographs for cases. Measurement of the ulcers area were evaluated by LesionMeter application.

Results. In the 1st group complete wound purification by the 2 weeks was observed in 90.91% of patients, in the 2nd group - in 86.96%. Statistically significant differences in the healing process rate were not observed between both groups in 2 weeks. Epithelization rate more than 50% was estimated as a criteria of efficacy in the term of 4 weeks. It was reached in 86.96% of the patients in the 1st group, and in 56.52% of the patients of the 2nd group. Unlike the 2nd group, the active formation of epithelization islets was observed over the entire surface at 22.73% in the 1st group.

Conclusions. It was demonstrated that including PDT in the complex treatment leads to local immune system activation with acceleration complete wound purification on the early stage of wound healing. At the same time the best result in the epithelization was obtained with PDT in patients of the 1st group. It’s can be explained by the formation of epithelium islets over the entire surface of ischemic ulcer in comparison with the regeneration of peripheral edges in the neurotrophic ones.

IN SILICO APPROACHES IN DRUG DESIGN OF NOVEL ANTIOXIDANT AGENTS

Olena Klenina, Volodymyr Ogurtsov, Borys Zimenkovsky
Danylo Halytsky Lviv National Medical University, 69 Pekarska Str., Lviv 79010, Ukraine
e-mail : olena_klenina@yahoo.com

The challenge of equally importance in modern medicine and pharmacy is the chemical regulation of numerous pathological conditions caused by the development of oxidative stress in a living organism. Increased interest in the establishment of preventive and therapeutic antioxidant of synthetic origin determines the relevance of developing and improving methods for antioxidant activity screening. Thiazolidine core is a powerful and effective pattern for rational design of "drug-like" molecules.

QSAR analysis for the antioxidant activity of 32 N^3 substituted 3*H*-thiazolo[4,5-*b*]pyridine-2-ones was performed. It was determined that antioxidant activity of the compounds depends mainly on descriptors that determine two-dimensional (2*D*) and spatial (3*D*) structure of their molecules. Six three-variables QSAR models were obtained. The interpretation of these models shows that the free radical scavenging activity of compounds increases with the presence of certain functional groups and structural fragments in their molecules, in particular, the structural fragments with the sum of topological distances equal to 2 and 5 with heavy terminal atoms enhance their antioxidant activity, while similar fragments presence with the sum of topological distances equal to 4 is undesirable. The presence of SPAN geometrical 3*D* descriptor and BEHm8 Burden eigenvalue matrice 2*D* descriptor in derived models ensures that free radical scavenging activity increasing corresponds to small molecules with the minimal distance of certain atoms and fragments from the center of mass and to the molecules without heavy atoms, the electronic density redistribution between the distant atoms and groups of atoms should be neglectable. The linear relationship between the activity and 3*D* molecular distribution of atomic masses in spherical volume with the radius of 13.0 Å was also proved. Some symmetry rules should be complied in the molecules of potent antioxidants namely strong symmetry of atoms with high electronegativity along the axis of the first component should be observed. The activity would also increase when each pair of heavy atoms will posess a low ability to interact, in particular, this may be possible if the heavy atoms would locate on opposite sides of the center of the molecule. The antioxidant activity of the compounds also increases with hydrophilic properties of the substances increasing.

It had been demonstrated that high statistical quality and predictive ability of the QSAR models obtained certify the possibility of their further application for the virtual screening of compounds libraries for identifying novel antioxidant agents based on the same congeneric series.

STRUCTURAL CHARACTERIZATION, ELECTROMAGNETIC AND THERMODYNAMIC PROPETRIES OF POULTRY BY-PRODUCTS

M. M. Zablodskij, S. I. Kovalchuk
[a]*National university of life and environmental sciences of Ukraine, str. Heroyiv oborony, 12, Kyiv, 03041, Ukraine*
e-mail: Stas_Kovalchuk@outlook.com

A growing need for sustainable and safe bio-based materials due to rising environmental concern has forced the use of available natural by-products as a substitution. Chicken feathers a waste material are a cheap, biodegradable and natural biopolymer produced in large amounts from poultry industries. Chicken feathers are mainly composed of the keratin is a biopolymer with a high degree of cysteine cross-linking [1]. Recently researchers have found potential applications of waste feathers by converting them into biodegradable polymers for expending the industrial applications [2].

The primary objective of this work is the investigation of structural characterization, electromagnetic and thermodynamic properties of the chicken feathers.

The investigation provides for a solution of numerical analysis and mathematical modelling thermodynamic and electromagnetic properties of chicken feathers in the processing of hydrothermal hydrolysis in a thin layer of raw under pressure. All stages of feather processing are performed in a twin-screw electromechanical hydrolyzer based on a polyfunctional electromechanical converter. Mathematical modelling is done in the «Python» programming language with integrating into «ANSYS» software. As a result of modelling, biologically significant physicochemical mechanisms of action on the substrate were determined, in particular, the influence of electromagnetic fields. Due to the processes in the wet down-feather mixture, thermal energy is generated, which can be determined through the mechanical energy component of the electromechanical hydrolyzer: $Q = 3{,}6 \cdot 10^3 \cdot N$ kJ. The picture of step-way change rheological properties of the down-feather mixture during processing in protein concentrate was defined.

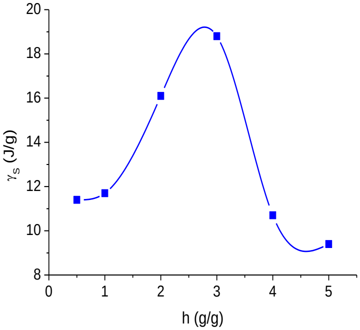
1. J. McKittrick, P-Y. Chen, S. Bodde, W. Yang, E. Novitskaya, M. Meyers. The structure, functions, and mechanical properties of keratin. *JOM*. 2012. № 64(4). Pp. 449–468.
2. Z. Shi, N. Reddy, X, Hou, YQ. Yang . Tensile properties of thermoplastic feather films grafted with different methacrylates. *ACS Sustain Chem Eng*. 2018. №2(7). Pp. 1849–1856. https://doi.org/10.1021/sc500201q.

INTERPHASIC INTERACTIONS IN MIXTURES OF HYDROPHOBIC AND HYDROPHILIC SILICA

V.V. Turov, T.V. Krupskaya, M.T. Kartel

Chuiko Institute of Surface Chemistry of National Academy of Sciences of Ukraine,
17General Naumov Str, Kyiv, 03164, Ukraine
e-mail: krupska@ukr.net

It is known that hydrophobic particles interact with the aqueous medium by means of van der Waals forces, and the state of the colloidal system strongly depends on the concentration of the dispersion medium. If the volume of water does not exceed the total volume of interparticle gaps in the aggregates, then water can be localized only in the porous silica system, and the air phase has a small effect on the relative position of the particles. An increase in the amount of water and the formation of a bulk phase of water that is not associated with silica increases the likelihood of dispersing solid particles in water. Therefore, the aim of the work was to determine the energy of interaction of water with the surface of a composite system containing equal amounts of hydrophilic and hydrophobic silicas. As the main research method, low-temperature 1H NMR spectroscopy was chosen.



It was shown that individual aggregates of the composite, and their hydrophilic and hydrophobic particles, become more mobile under the influence of mechanical stress, and can be positioned in such a way as to ensure the minimum value of the free energy of the colloidal system, which corresponds to the maximum binding of interfacial water and the maximum value of interfacial energy (figure). When passing into the region of concentrated aqueous suspensions (4000-5000 mg/g), due to the contact of the suspension with air, partial replacement of water with air in hydrophobic cavities of the composite particles can be carried out. This process is accompanied by a decrease in the contact zone of the solid surface of the composite with water, and, consequently, leads to a decrease in the interfacial energy of the particle-water.

As a result of the work, it was found that the dependence of the energy of interaction of water with the surface of the particles of the composite system, created on the basis of hydrophilic and hydrophobic silicas, has a bell-shaped appearance with a maximum at a hydration of 3000 mg/g. Under the influence of mechanical stress in the initial stages of hydration, the air in the interparticle gaps of the composite is replaced by water. With high hydration, it is possible to rearrange the relative positions of hydrophobic and hydrophilic particles, accompanied by an increase in the interaction energy with the aqueous medium. A further increase in hydration leads to a partial replacement of water in the interparticle gaps of the hydrophobic component with air, which entails a decrease in the value of interfacial energy.

USE OF PHOTODYNAMIC THERAPY FOR TREATMENT OF CHRONIC ULCERS

B. V. Krysa, V. M. Krysa
Ivano-Frankivsk National Medical University
2 Halytska Str., Ivano-Frankivsk, 76018, Ukraine.
E-mail: bodja.ua@gmail.com

Treatment of chronic ulcers is one of the oldest medical issues which remain topical until nowadays and constantly demand development of efficient methods.

Objective. Analysis of impact of low-power laser radiation with wavelength of 660 nM on repair of chronic ulcer skin defects.

Materials and methods. Photodynamic therapy was applied to 29 patients aged 36–67 with venous (22) and diabetic ulcers (7). 1 % solution of methylene blue was applied to tissues which were then radiated by Lika-terapevt device (50–70 mW, dosage of 6–8 J per 1 cm^2). Ulcers were covered with wet-to-dry antiseptic-containing dressing and after beginning of epithelialization – with hydrophilic dressing.

Results. After 3 to 4 procedures, the ooze volume reduced, ulcers were covered by granulation tissue, in 5 to 6 sessions, marginal epithelialization was revealed. It was a sign for cancelling the laser treatment to prevent inhibition of reparative processes.

Conclusions. Monochromatic 660 nM laser radiation combined with local photosensitization with a 1 % solution of methylene blue facilitates repair of ulcers resistant to traditional treatment methods.

IN VITRO RESEARCH ON DEGRADATION OF 60S BIO-CERAMIC IMPLANT MATERIALS

Kusyak A.P.[a], Chornyi V.S.[b], Dubok V.A.[c],
[a] *Ivan Franko Zhytomyr State University, 40 V. Berdychivska Str., Zhytomyr, 10008, Ukraine*
[b]*Bogomolets National Medical University, 13 Tarasa Shevchenko Blvd, Kyiv, 01601, Ukraine*
[c]*I.M. Frantsevich Institute for Problems of Materials Science, NAS of Ukraine, 3 Krzhizhanovsky str., Kyiv, 03142, Ukraine*
e-mail: a_kusyak@ukr.net

One of the bone grafting materials is 60S sol-gel glass which is characterized by osteoproductive and osteoconductive properties. An in vitro study allows us to evaluate the sorption and resorption properties of materials. Creation of a 60S sol-gel glass implant with specified antibacterial, chemotherapeutic properties of prolonged local action for a drug delivery system is promising for the use in bone tissue engineering in orthopedics. The aim of the study is to investigate the features of ion exchange processes of 60S sol-gel glass in a model biological environment, to study the possibility of adsorbing immobilization of antibacterial drugs on its surface.

The sol-gel synthesis method produced samples of 60S glass (4% P_2O_5, 36% CaO and 60% SiO_2) (1) and doped with Ga (1%) (2), Ge (1%) (3) and collagen type 1 (4). The dissolution processes in the model biological environment - SBF solution (Kokubo model) are investigated. Changes in the ionic composition of SBF solution during the dissolution of glass in the dynamic mode were investigated by atomic absorption method, the pH of the medium was controlled by a potentiometric method.

The processes of ion exchange of glass with protons of SBF solution and the hydration reaction lead to an increase in the pH of the medium (up to 8.5) in all samples. The concentration of OH ions is not high enough to depolymerize the glass structure, but sufficient to activate the surface silanol groups that form the active sorption centers. The investigated samples are characterized by active sorption processes involving Mg^{2+} ions. For Ca^{2+} ions, on the contrary, release processes predominate. For HPO_4^{2-} ions, which form a hydroxapathy-like surface layer, active sorption processes are characteristic of samples 1, 2, desorption sorption for sample 3, and virtually no sorption processes for sample 4. It should be noted that in this time range the processes are not fixed. of the reverse sorption of Ca^{2+} ions, which indicates the active degradation and formation of the silicate-helium layer necessary for the formation of calcium phosphate film, which is a condition for the formation of the biologically active layer of hydroxoapatite - an ideal environment for adsorption its growth factors and cell attachment, proliferation and differentiation of cells.

Active exchange processes with the model environment indicate the prospect of studies of synthesized 60S glass samples as implant materials.

NANOCOMPOSITES FOR ANTICANCER THERAPY

Nataliya Kutsevol[1], Yuliia Kuziv[1], Vasyl Chekhun[2], Vladimir Zorin[3], Michel Rawiso[4]

[1]Taras Shevchenko National University of Kyiv, 60 Volodymyrska str., 01602 Kyiv, Ukraine;
e-mail: kutsevol@ukr.net
[2] R.E. Kavetsky Institute of Experimental Pathology, Oncology and Radiobiology, 45 Vasylkivska str., 03022 Kyiv, Ukraine
[3]Belarussian State University, pr. Nezavisimosti 4, Minsk, 220030 Belarus
[4] Institute Charles Sadron (CNRS-UdS), 23 Loess str., Strasbourg 67034, France

Multicomponent nanocomposites for anticancer therapy were prepared and characterized. The water-soluble star-like dextran-graft-polyacrylamide copolymer was used as a nanoplatform for the creation of polymer-based multicomponent drug delivery systems for photodynamic and combined (photodynamic+chemotherapy) antitumor therapy. The three-component nanocomposites with incorporated gold nanoparticles and photosensitizer and the four-component ones additionally loaded by Doxorubicin into polymer nanoplatform were studied at 25 and 37 ºC by Transmission electron microscopy and Dynamic light scattering. Nanocomposites were tested for their photodynamic cytotoxicity for the cell line of breast cancer MCF-7/S. A semiconductor laser (PMNP Photonic Plus, Cherkasy) with a wavelength of 660 nm, which coincides with one of the Ce6 absorption maxima, was used as a light source for photodynamic damage to cells.

In the "control" experiment the cancer cells were subjected to the same manipulations but without the addition of nanocomposites. It was shown that MCF-7/S cells were not sensitive to all Nanocomposites without external irradiation.

It was found that three-component nanocomposites demonstrated higher efficacy than the four-component ones. It was explained by the aggregation process provoked by adding of additional component resulted in decreasing of a hydrophilic-hydrophobic balance of polymer macromolecule.

Acknowledgment

This publication is supported in part by the Ministry of the Education and Science of Ukraine: joint Ukrainian-Belarusian research and development projects "Design and physico-chemical properties of novel multicomponent nanosystems for the treatment and diagnostics of solid tumors" M/110 (2019-2020), and with the financial support of the Belarusian Republican Foundation for basic research, grant no. M19UKRG-002.

ENHANCEMENT OF THE X-RAY PDT NANOSYSTEM EFFICIENCY BY THE PRESENCE OF HfO_2 NANOPARTICLES

Losytskyy M.Y.[a], Vretik L.O.[a], Nikolaeva O.A.[a], Degoda V.Y.[a], Shcherbakov O.B.[b], Podust G.P.[a], Doroshenko I.P.[a], Ohulchanskyy T.Y.[c], Yashchuk V.M.[a]
[a] *Taras Shevchenko National University of Kyiv, Volodymyrs'ka Str., 64/13, Kyiv-01601, Ukraine*
e-mail: mlosytskyy@univ.kiev.ua; mlosytskyy@gmail.com
[b] *Zabolotny Institute of Microbiology and Virology, NAS of Ukraine, Kyiv, Ukraine*
[c] *College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, Guangdong Province, 518060, P. R. China*

Photodynamic therapy (PDT) is the method of cancer treatment that involves photosensitizer (PS) molecules which accumulate in tumor and, after excitation with light, use the excitation energy to generate toxic reactive oxygen species. To overcome the problem of low depth of light penetration into human body, X-ray PDT was proposed that employs deeply penetrating X-rays instead of visible or NIR light. To be used in X-ray PDT, nanosystems consisting of scintillator part (that absorbs high-energy X-ray quanta and transforms them into low-energy electronic excitations) and PS part are being developed, with excitation energy transfer from the former to the latter one [1]. Recently, we have designed and studied the nanosystem consisting of polystyrene nanoparticle with incorporated molecules of diphenyloxazole (PS-PPO NP) as scintillator and chlorin e_6 as PS, excitation energy transfer from polystyrene matrix through PPO to chlorin e_6 was demonstrated [2]; X-ray stimulated luminescence of PS-PPO NP was also observed [3]. To demonstrate the possibility to enhance the efficiency of such nanosystem by non-emitting heavy elements, here we report the effect of HfO_2 nanoparticles on the X-ray stimulated luminescence of PS-PPO NP. Thus, excitation with the X-rays (energy of quanta about 15 keV) of the colloidal suspension of PS-PPO NP (about 8% by mass) in the presence of HfO_2 nanoparticles (about 1.25% by mass) resulted in the luminescence emission of PPO that was 15% more intense than the X-ray stimulated PPO emission from the analogous PS-PPO NP sample without HfO_2 nanoparticles. We believe that this result is attributable to the additional excitation of styrene matrix of PS-PPO NP by secondary electrons emitted after X-ray excitation of heavy Hf atoms. This result could be further used in the development of sensitizing nanosystems for X-ray PDT.

[1] W. Fan, P. Huang, X. Chen. *Chem. Soc. Rev.*, **2016**, 45, 6488-6519.

[2] M.Yu. Losytskyy, L.O. Vretik, O.A. Nikolaeva, A.I. Marynin, N.F. Gamaleya, V.M. Yashchuk. *Mol. Cryst. Liq. Cryst.*, **2016**, 639, 169-176.

[3] M. Losytskyy, L. Vretik, O. Nikolaeva, D. Getya, A. Marynin, V. Yashchuk. *French-Ukrainian Journal of Chemistry*, **2015**, 3(2), 119-124.

EVALUATION OF ACID-BASE SURFACE PROPERTIES OF NANOSCALE Fe_3O_4 BY POTENTIOMETRIC TITRATION

Kusyak N.V.[a], Kusyak A.P.[a], Petranovska A.L.[b], Gorbyk P.P.[b],
[a] *Ivan Franko Zhytomyr State University, 40 V. Berdychivska Str., Zhytomyr, 10008, Ukraine*
[b] *Chuiko Institute of Surface Chemistry of National Academy of Sciences of Ukraine,*
17 General Naumov Str., Kyiv, 03164, Ukraine
e-mail: nkusyak@ukr.net

The interest in single-domain magnetite (Fe_3O_4) nanoparticles on the basis of is due to the fact that these nanoparticles are characterized by the unique combination of physical, chemical, and biological properties, satisfactory biodegradation and possibility of production of ferrofluids on their basis. The chemical activity and sorption characteristics of a surface depend on active centers quantitative and quality indicators. Researches of nature of acid-base properties allows to optimize conditions when developing materials of purpose.

The objective of the present study is to elucidate and investigate the acid-base properties Fe_3O_4 surface in the environment of saline. Nanodispersed magnetite was synthesized by the co-precipitation of iron salts by the reaction $Fe^{2+} + 2Fe^{3+} + 8NH_4OH \rightarrow Fe_3O_4 + 4H_2O + 8NH_4^+$. The average diameter of the nanoparticles calculated by the results of studies of X-ray diffractograms using the Scherrer formula was 10.5 nm, the specific surface area measured by the method of nitrogen desorption, Ssp = 110 ± 1% m^2/g. In the study of the infrared spectra of the surface of the magnetite revealed functional OH-groups, the concentration of which according to thermogravimetric analysis of 1.8 mmol/g. The synthesized magnetite is characterized by satisfactory magnetic characteristics: the coercivity Hc = 55.0 ± 2.5% Oe, the specific magnetization of saturation σs = 56.2 ± 2.5% Gs cm^3/g, relative residual magnetization Mr/Ms = 0.2 ± 2.5% [1]. These characteristics meet the requirements for medical and biological nanoparticles.

The acid-base properties of the surface of the samples were investigated by the method of pH-metry, which allows to evaluate the integral acidity of the surface when studying the change in the pH of the aqueous suspension of the samples. Groups with different ionization constants have been found on the surface, which is related to differences in the coordination of ferum atoms with oxygen atoms, crystal lattice defects, and the degree of surface group hydration. The obtained data on the level of surface isoadsorption state (pH_{pzc}), ionization constants of active centers by acid and basic mechanisms, diagrams of distribution of active centers depending on pH, and quantified the concentration of acid-base active centers of the surface.

[1] Petranovska A.L., *Chemistry, Physics and Technology of Surface*, **2019**, 10(4), 419-431.

GREEN SYNTHESIS AND ADSORPTION PROPERTIES OF COBALT FERRITES

M. Liaskovska[1,2], T. Tatarchuk[1,3]

[1]Department of Chemistry, Vasyl Stefanyk Precarpathian National University, 57, Shevchenko Str., Ivano-Frankivsk, 76018, Ukraine

[2] H.O. Babenko Department of Biological and Medical Chemistry, Ivano-Frankivsk National Medical University, 2 Halytska Str., Ivano-Frankivsk, 76018, Ukraine

[3]Educational and Scientific Center of Materials Science and Nanotechnology, Vasyl Stefanyk Precarpathian National University, 201, Galytska Str., Ivano-Frankivsk, Ukraine

e-mail: tatarchuk.tetyana@gmail.com

Materials with spinel structure have long been a topic of interest because they exhibit different properties depending on synthesis method. In this research, we have used the green chemistry method for cobalt ferrites synthesis using of various plant extracts. The reducing capability of this plants is based on several reactive components such as polyphenols, terpenoids, amino acids etc.

Spinel type materials have long been a topic of interest because they may exhibit different sizes depending on synthesis method. In addition, they can be use as magnetic materials, pigments, catalysts and refractory materials. The aim of our research is to design an ecological method for the synthesis of magnetic nanoparticles with a high specific surface area. Spinel structure of magnetic nanoparticles has been confirmed by XRD and IR spectroscopy. The IR spectra contain two main peaks that correspond to tetrahedral and octahedral sites in spinel structure respectively, and few peaks in the range 1300-3700 cm^{-1} that shown surface functionalization of magnetic nanoparticles. The surface morphology and elemental composition were proved by using SEM and EDS respectively. The synthesized cobalt ferrites were investigated as magnetic adsorbents using anionic dye Congo red as model pollutant. In addition, the $CoFe_2O_4$ nanoparticles obtained by eco-friendly method using plant extract as chelating agent could be used as good candidate for biomedical applications, such as drug delivery and hyperthermia application.

BINDING OF Zr PHTHALOCYANINES WITH BETA-LACTOGLOBULIN: SPECTRAL-FLUORESCENT STUDY

Losytskyy M.Y.[a], Chernii S.V.[a], Chornenka N.V.[b], Tretyakova I.M.[b], Chernii V.Y.[b], Kovalska V.B.[a]

[a] *Institute of Molecular Biology and Genetics NASU, Zabolotnogo Str. 150, Kyiv, 03680, Ukraine*

e-mail: mlosytskyy@gmail.com

[b] *V.I. Vernadsky Institute of General and Inorganic Chemistry NASU, Palladina Ave. 32/34, Kyiv, 03142, Ukraine*

Amyloid aggregation is the process of proteins misfolding, where denatured protein molecules bind together and form rigid insoluble structures named amyloid fibrils. This process is mostly known to accompany neurodegenerative deceases (e.g. Alzheimer’s or Parkinson’s diseases), but takes place also in several other cases, one of them is the food processing. Particularly, beta-lactoglobulin (BLG) is an important protein of milk whey and, on the other hand, is known to form amyloid aggregates. Since amyloid aggregates of BLG should be avoided in food, the ways of inhibition of such aggregation should be studied. One of the approaches to inhibit the formation of amyloid aggregates is to form complex between the inhibitor ligand molecule and the native form of the protein (e.g. monomer, dimer or hexamer). As model ligands to study the formation of such complexes, phthalocyanines could be used; compounds of this class were previously reported as compounds able to stabilize protein conformation and efficiently inhibit amyloid aggregation of proteins.

Here we studied the interaction of BLG in 50 mM Tris-HCl buffer (pH 7.9) with zirconium phthalocyanines containing two chlorine atoms ($PcZrCl_2$) and two citric acid residues ($PcZrCitr_2$) as out-of-plane ligands. The study of absorption spectra showed the difference in the shape of the spectra of phthalocyanines in the presence of BLG and in its absence. Besides, it was shown that the presence of BLG leads to the increase in the fluorescence intensity of both phthalocyanines. These observations point to the interaction of both $PcZrCl_2$ and $PcZrCitr_2$ with BLG in water solution. At the same time, fluorescence excitation spectra showed the absence of excitation energy transfer from tryptophan residues of BLG to phthalocyanines. Thus, phthalocyanines bind to BLG at either big distance or perpendicular orientation of transition dipole moments with respect to its tryptophan residues (or both these factors). Finally, the measured dependence of phthalocyanines fluorescence intensity on BLG concentration gave possibility to estimate the equilibrium constant (K_b) of phthalocyanines binding to BLG; these values were estimated as $K_b = (2.4\pm0.6)\times10^5$ M^{-1} for $PcZrCl_2$ and $K_b = (1.2\pm0.14)\times10^5$ M^{-1} for $PcZrCitr_2$. Thus, the studied phthalocyanines $PcZrCl_2$ and $PcZrCitr_2$ could be further investigated as model inhibitors of BLG amyloid aggregation.

The study was supported by CRDF Global grant #65501.

LIGHT-INDEPENDENT PRO-OXIDANT ACTIVITY OF UV PRE-IRRADIATED ORTHOVANADATE NANOCRYSTALS

Pavel Maksimchuk, Valeriia Omielaieva, Kateryna Hubenko, Vladyslav Seminko, Svetlana Yefimova, Yuri Malyukin
Institute for Scintillation Materials NAS of Ukraine, 60 Nauky Ave., Kharkiv 61072, Ukraine
e-mail: pmaksimchuk@isma.kharkov.ua

The ability of dielectric nanoparticles to generate reactive oxygen species (ROS) under X-ray excitation enhances sufficiently the efficiency of cancer radiotherapy making such nanoparticles a promising material for biomedical applications. However, the ionizing radiation used during radiotherapy has a great disadvantage of being dangerous not for cancer cells only, but for whole organism as well. For solving this problem, we propose orthovanadate nanocrystals with light-independent pro-oxidant activity without any external stimuli after pre-irradiation of nanoparticles with UV-light [1].

Light-independent pro-oxidant activity of orthovanadate nanoparticles is shown to be associated with superoxide and hydroxyl radical generation and depended on the size of nanocrystals and, consequently, on the concentration of surface defects [2]. Oxide nanoparticles contain high amount of structural defects (such as oxygen vacancies) which could serve as traps for charge carriers and are responsible for ROS production in nanocrystals even long time after irradiation. For small 2 nm orthovanadate nanoparticles, strong superoxide and hydroxyl radical production has been revealed, whereas for larger orthovanadate nanocrystals, low level of superoxide and negligible one of hydroxyl radicals production have been detected during the storage of the samples in the darkness.

Orthovanadate nanocrystals with light-independent pro-oxidant activity could be prospective for the application in biomedical area as multifunctional therapeutic agents for cancer treatment.

[1] S.L. Yefimova, P.O. Maksimchuk, K.A. Hubenko, V.K. Klochkov, A.V. Sorokin, Yu.V. Malyukin. *Colloids and Surfaces A.* **2019,** 577, 630-636.

[2] Pavel O. Maksimchuk, Svetlana L. Yefimova, Kateryna O. Hubenko, Valeriia V. Omielaieva, Nataliya S. Kavok, Vladimir K. Klochkov, Alexander V. Sorokin, Yuri V. Malyukin. *Phys. Chem. C.* **2020**, in press.

HYBRID HYDROGELS LOADED WITH BIOLOGICAL ACTIVE DYES AS MATERIALS FOR THERAPEUTIC DELIVERY

Nadtoka Oksana[a], Virych Pavlo, Kutsevol Natalia, Martynyuk Victor
[a] *Taras Shevchenko National University of Kyiv, 64/13, Volodymyrska Street, Kyiv 01601, Ukraine*
e-mail: oksananadtoka@ukr.net

Hydrogels are network of polymer chains, which can swell in aqueous solutions, hold a large amount of water, permeate to oxygen and nutrients. They can be used in the fields of implantable artificial organs, drug delivery, cell encapsulation, toxic ion removal, and wound dressing for therapy in a humid environment. The sorption capacity during sorption/desorption cycles is an important characteristic of hydrogels used in the removal of contaminants from the wounds. At the same time, wound healing requires a sterile medium with prolonded drug delivery.

To enhance the mechanical strength and sorption/desorption response, hybrid polymer networks of Dextran-graft-Polyacrylamide (D-g-PAA) have been designed. The main advantages of D-g-PAA are that relatively structured hydrogel matrices can be produced, which possess more widely controllable physical properties, and (frequently) more efficient drug loading compared to single-network hydrogels.

The sorption/desorption capacity of Dextran-graft-Polyacrylamide hydrogels in the presence of ionic dyes has been evaluated. The most well-known and versatile biologically active dyes methylene blue, diamond green, alkaline fixin were used for the study.

It was studied, that the sorption equilibrium has been attained faster and loading capacity of the of cross-linked D-g-PAA significantly increased compared to pure cross-PAA hydrogel. Sorption/desorption properties of hybrid hydrogels were studied by estimating the change in the absorption maximum of MB solutions. It was obtained that sorption/desorption rate of dyes into/out off hydrogel depends on the hydrogel structure. The antibacterial properties of hybrid hydrogels loaded with biological active dyes were tested against *Staphylococcus aureus*. The satisfactory antimicrobial efficacy was registered for dye-loaded hydrogels in humid environment.

So, by applying the strategy of synthesis of hybrid polymer networks the diffusion of drugs out of hydrogel matrices has been improved.

CHRONIC VENOUS DISEASE CEAP 1-2 TREATMENT WITH 1064 Nd:YAG LASER

Viktoriia Mishura, Yurii Melekhovets, Vasyl Pak, Oksana Melekhovets, Oleksandr Sytnik
Sumy State University, 2 Rymskogo Korsakova, 40007 Sumy, Ukraine
e-mail: vikamisura153@gmail.com

Background. The problem of chronic venous disease (CVD) remains relevant to this day, despite the significant progress from the first descriptions of the disease to the introduction of the newest methods of its treatment. This is due to its widespread prevalence in the world, the impact on the working population, the worsening of the quality of life of patients, as well as the socio-economic influence of the disease. CVD early stages treatment is aimed in restoring of the aesthetic comfort, in particular – at the elimination of the existing cosmetic defects and prevention of new ones.

The aim - to evaluate the safety and efficacy of 1064-nm Nd:YAG laser in the treatment of C1-2 clinical stages of the chronic venous disease.

Methods. The study randomly included 60 patients with telangiectasia and small varicose veins less than 4 mm in diameter. Based on the diameter of the vessels (d<1mm (n = 22), 1-2mm (n = 20), 2-4mm (n = 18)), the patients were divided into 3 groups. They were comparable in age (46±8), gender (mostly women in all groups – 90-92%) and clinical status. The following methods were applied: objective examination of the local status treatment area photos, ultrasound monitoring with SonoScape S6 with linear transduser L741, subjective evaluation of the results of treatment by the patient, statistical analysis. Treatment efficiency and complications were monitored in 2 weeks and in 3 months after the procedure.

Results. Treatment area photos in 2 weeks demonstrated improvement in small varicose veins and telangiectasia appearance. This improvement persisted over a 3-month follow-up, indicating the long-term effect of the treatment. No significant adverse events were observed as a result of the treatment. Most of the complications (pain during the procedure, incomplete disappearance of vessels, relapse) were obtained in the treatment of veins with d=2-4mm. The same time, the best subjective result (100%) and objective result (the percent of reduction in the severity of veins after laser treatment >75%) (95,5%), were obtained in the treatment of veins d<1 mm. The influence of the laser on veins with d=1-2mm had a positive objective 80% result.

Conclusion. The 1064-nm Nd:YAG laser is the safe and effective option for the treatment of small varicose veins and telangiectasia up to 2 mm in size on the lower extremities.

RESEARCH OF WORK OF A ROOFTOP SOLAR POWER PLANT IN HOT WATER SUPPLY SYSTEMS OF STUDENT DORMITORIES

Nalyvaiko Vitalii, Radko Ivan, Okushko Oleksandr, Mrachkovska Nadiia
Antypov Ievgen
National University of Life and Environmental Sciences of Ukraine,
12, Heroyiv Oborony Str., Kiev, 0304, Ukraine
e-mail: nva041@ukr.net

Every year, about five-fifths of fuel and energy resources spent on the household needs of Ukraine's population, and prices are rising rapidly from year to year. In urban networks, hot water heats centrally, with about 30% of energy is lost in transit.

The purpose of the study is to improve the energy efficiency of the utility facilities.

We investigated a rooftop solar power plant with a maximum power of 30 kW. The rooftop power capacity is limited by a small roof area of a multi-stored building. Therefore, an industrial heat pump with a heat output of 95 kV uses for direct water heating. Such capacity is sufficient for hot water supply of a multi-stored city building with 600 people [1].

Hot water consumption is unstable and in many cases unpredictable. Moreover, the maximum consumption does not coincide with the maximum power of the solar power plant. Therefore, using the simulation methods, the required amount of buffer capacity of the hydro accumulator was calculated.

The microprocessor system based on the neural network regulates the operation of the hot water system. It allows maximum efficiency to use the power of solar panels, to take into account and adjust in real time the amount of consumed hot water, to take into account the weather forecast for the next day and to use the heat pump at night at reduced tariff price.

Economic calculations confirm the reduction of the cost of one m3 of hot water by 2-2.5 times compared to centralized water supply. In addition, the proposed system operates from renewable energy sources and does not pollute the atmosphere [2].

Reference

1. Radko I., Nalyvaiko, V., Okushko O. Improve the energy efficiency of heat supply systems in educational institutions. Scientific bulletin of the Tavria State Agrotechnological University. 2019, Vol. 9, Iss. 1, journal-articl
2. Radko I., Nalyvaiko, V., Okushko O., Mishchenko A., Antypov Ie. Investigation of ways of reducing heat losses in NULES of Ukraine. Power engineering and automation. 2019, Vol. 1. P. 114-126.

SYNTHESIS OF POLYMERIC HYDROGELS INCORPORATING CHLORHEXIDINE AS ANTIBACTERIAL WOUND DRESSINGS

Oksana Nadtoka[a], Pavlo Virych[a], Vasyl Krysa[b], Nataliya Kutsevol[a]
[a]*Taras Shevchenko National University of Kyiv, 64/13, Volodymyrska Street, Kyiv 01601, Ukraine*
[b]*Ivano-Frankivsk National Medical University, Galytska str., Ivano-Frankivsk 76000, Ukraine*
e-mail: oksananadtoka@ukr.net

Nowadays, there are various types of wound covering materials; however, each type has its unique characteristic for a specific wound. A wound dressing for improving wound healing process is a challenge for medical device in recent years. Several researches have been accepted that a moist dressing is able to promote and accelerate the wound healing process when compared with dry dressing because moist environment renewed skin without eschars formation and inflammation. However, there is a disadvantage of the moist environment as it could promote bacterial growth leading to increase the risk of wound infection. To overcome this drawback, hydrogels were fabricated the structure of hydrogels could be designed to possess antibacterial behaviors or incorporated with the antibacterial agents.

Antibacterial hydrogels based on Dextran-graft-Polyacrylamide and Dextransulfate-graft-Polyacrylamide loaded by chlorhexidine (CH) as a drug were fabricated (Fig.1). Dextran and Dexstransulfate Na salt were used for synthesis for obtaining nonionic and ionic polymer network. It was shown, that strongly ionizable-sulfonate groups contribute to high water absorption capability of the hydrogel (Fig.1) as well as will affect the hydrogel structure.

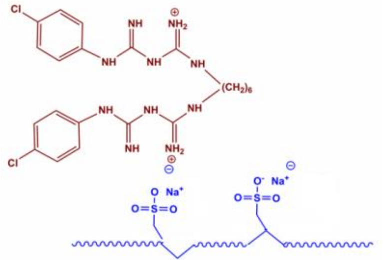


Figure 1.

Chlorhexidine is an antiseptic and anti-inflammatory agent providing a wide range of efficient resistance, including gram-negative and gram-positive bacteria. Interaction between hydrogel matrices and chlorhexidine were studied by FTIR-spectroscopy. Chromatography analysis was used for determination of CH concentration in polymeric hydrogels.

The hydrogel was examined for sorption-desorption capacity toward of CH. It was found that that the CH strongly interacted with the hydrogel network. The antibacterial efficiency of the hydrogels was tested by using disc-diffusion method on a Müller-Hinton agar. The ability of hydrogels to inhibit bacterial growth the *Staphylococcus aureus* strains obtained on Endo media and Yolk-salt agar were used. The prepared hydrogels loaded by CH demonstrated their potential for using as wound dressing with antibacterial efficacy.

NANOPARTICULAR AGENTS FOR NEAR INFRARED LUMINESCENCE BIOIMAGING AND IMAGING GUIDED THERAPY

T.Y. Ohulchanskyy
College of Physics and Optoelectronic Engineering, Shenzhen University, Shenzhen, Guangdong, 518060, People's Republic of China
e-mail: tyo@szu.edu.cn

Nanotechnology advances biomedical field by introduction of multimodal imaging probes and nanoplatforms for enhanced, targeted therapy. Imaging guided nanovehicles for drug delivery are among the most intensively developed subjects in the medical application of nanotechnology. With the nanochemistry-enabled combination of diagnostics and therapeutics approaches, a nanoscale theranostics is arising, providing a powerful paradigm for a modern personalized medicine.

In the last few years, we have been working on inorganic and organic nanomaterials for optical bioimaging and imaging guided phototherapy. Light induced electronic processes play a key role in the functionality of these photoactive nanoplatforms; their imaging and therapeutic modalities can be tuned and optimized through the control of the excitation dynamics and specific electronic processes within nanoparticles. On the other hand, theranostic applications of light are greatly determined by its ability to penetrate a tissue, which is known to be higher in near- and short wave infrared (NIR-SWIR) regions of the electromagnetic spectrum. This talk will present our recent results on development of heterogeneous nanoparticles which can be detected/imaged in vitro and in in vivo through their NIR-SWIR luminescence. In addition to the luminescence imaging contrast, nanoparticles can be equipped with the phototherapeutic modalities and the talk will provide examples of the nanoformulations, where electronic processes have been orchestrated to enhance imaging and therapeutic functionalities. The developed nanostructures include liposomal and polymeric nanoparticles and rare-ion doped nanophosphors, as well as their combinations with near-infrared fluorescent organic dyes and other functional small molecules.

While possessing the luminescence imaging contrast and therapeutic functionality, the light active nanoplatforms can be also garnished with other medical imaging modalities, enabling the integration of cellular, tissue and whole body imaging and providing a single nanoagent for multiple imaging techniques. The talk will demonstrate examples of applications of nanoparticles as multimodal imaging guided theranostic agents and conclude with a discussion on the challenges and opportunities in the domain of NIR-SWIR luminescent nanoformulations for imaging guided phototherapies of cancer and other diseases.

PHOTOINACTIVATION OF *STAPHYLOCOCCUS AUREUS* WITH MONOCHROMATIC LOW ENERGY VISIBLE LIGHT

Pavlo Virych[a], Oksana Nadtoka[a], Petro Virych[b], Victor Martynyuk[c], Nataliya Kutsevol[a]
[a]*Taras Shevchenko National University of Kyiv, Faculty of Chemistry, Lva Tolstogo str. 12, Kyiv, 03033, Ukraine*
[b]*SE “Kolomiychenko Institute of Otolaryngology of the National Academy of Medical Sciences of Ukraine”, Zoologichna str. 3, Kyiv, 03680, Ukraine*
[c]*Taras Shevchenko National University of Kyiv, Educational and Scientific Centre "Institute of Biology and Medicine", Glushkova av. 2, Kyiv, 03022, Ukraine*
e-mail: sphaenodon@ukr.net

The wide spread use of antibiotics for the treatment of bacterial diseases has reduced a mortality rate of a population. However, at the same time there are strains that are not sensitive to the antibiotics action. In contrast to antibiotics, visible light has a wide range of bactericidal action and can be used without risks when take place an intentional illumination of human tissue. The functions of endogenous photosensitizers can be performed by hemoporphyrins, flavoproteins, heterocyclic compounds and other substances that absorb certain parts of the spectrum [1]. We investigated *in vitro* photoinactivation of wild strains of *Staphylococcus aureus*. The bacteria were incubated at 37 °C in the Müller-Hinton liquid medium (g/l): casein hydrolyzate - 17.5, bovine heart hydrolyzate - 2, starch - 1.5, pH = 7.3. The suspension was irradiated with monochromatic light at 390 nm, 460 nm, and 530 nm wavelengths. The output energy of each wavelength was 0.1 J/s. The dose of irradiation was in the range between 1-18 J/cm^3. Bacteria photoinactivation efficiency of each experimental variant was compared with a parallel sample. After irradiation bacterial suspension was dyed with 0.001% acridine orange during 5 min. The number of colonies forming units (CFU) was calculated in Goryaev chamber. The maximum effect (about 65% of inactivation CFU) was obtained at 390 nm wavelength with an irradiation dose of 18 J/cm^3. In case of further increasing of an irradiation dose, the rising effect was remained. At 460 nm, the maximum effect (about 60% of inactivation CFU) was obtained at a dose of 10 J/cm^3, and 530 nm – at dose 6 J/cm^3 (about 50% of CFU inactivation). Further increase of the irradiation dose for both wavelengths does not increase the number of inactivated CFU.

We assume a non-specific effect of UV radiation (390 nm). The 460 nm and 530 nm wavelengths may have intracellular specific targets that can damage important cell components when activated. For blue light, these may be hemoporphyrins, which have main absorption maxima in this area. Green light is absorbed by flavoproteins. Both groups of compounds are important constituents of electron transport systems of microorganisms and are constitutively present in bacterial cells.

Thus, low energy monochromatic light with wavelengths of 390, 460, 530 nm are able to effectively inactivate wild strains of *Staphylococcus aureus*.

1 M. Hessling, B. Spellerberg, K. Hoenes. Photoinactivation of bacteria by endogenous photosensitizers and exposure to visible light of different wavelengths – a review on existing data. FEMS Microbiology Letters, 2017, V. 364, No. 2, p. 270.

FORMATION AND DYNAMICS OF OXYGEN VACANCIES IN CeO_2-ZrO_2 AND CeO_2-Y_2O_3 NANOCRYSTALS

Okrushko O., Seminko V., Maksimchuk P., Malyukin Yu.
Institute for Scintillation Materials, National Academy of Sciences of Ukraine,
60 Nauky Ave., Kharkiv, 61072,Ukraine
e-mail: elenaokrushko0501@gmail.com

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

The dependence of the processes of formation of oxygen vacancies on the content of yttrium and zirconium ions in CeO_2-ZrO_2 and CeO_2-Y_2O_3 nanocrystals was investigated. Luminescence spectra of both mixed nanocrystals consisted of the two bands determined by F-centers and 5d→ 4f transitions of Ce^{3+} ions (Ce^{3+} luminescence). Intensity of Ce^{3+} luminescence is significantly dependent on concentration of oxygen vacancies in nanocrystals. It was shown that increase of the concentration of yttrium and zirconium ions leads to an increase in the intensity of the Ce^{3+} luminescence band, which indicates an increase in the concentration of oxygen vacancies.

The luminescence of Ce^{3+} ions also makes possible to study the dynamics of the interaction of nanoceria and mixed cerium-yttrium or cerium-zirconium oxides with reactive oxygen species using spectroscopic techniques. Interaction of nanoceria with hydrogen peroxide leads to $Ce^{3+} \rightarrow Ce^{4+}$ oxidation accompanied by oxygen diffusion deep into the nanoparticle, and recovery ($Ce4^{+} \rightarrow Ce^{3+}$) occurred with by oxygen diffusion from the bulk to the surface and then out of ceria nanoparticle. It was shown that temperature increase facilitate recovery of initial Ce^{3+} luminescence intensity due to the increase in the rate of oxygen diffusion within nanoceria volume. The incorporation of yttrium and zirconium ions in nanoceria leads to faster diffusion on the oxidation stage ions and to slow-down of these processes on the recovery stage.

MASS SPECTROMETRY STUDY OF NANOBIOCOMPLEXES FORMATION BETWEEN DIMETHYL SULFOXID AND ANTIMICROBIAL AGENTS

V. Pashynska[a], M. Kosevich[a], A. Gomory[b]
[a] *B. Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine, Nauky Avenue 47, 61103 Kharkiv, Ukraine*
[b] *Institute of Organic Chemistry of Research Centre for Natural Sciences, Magyar tudosok korutja 2, Budapest, H-1117, Hungary*
e-mail: pashynska@ilt.kharkov.ua

Application of nanotechnologies for drugs delivery and understanding the role of nanobiocomplexes formation in molecular mechanisms of facilitating the transdermal and transmembrane medications transfer are urgent problems of the modern nanobioscience and molecular medicine. Having a significant experience in the soft ionization mass spectrometry technique usage for study of intermolecular interactions of biologically active compounds with targeting biomolecules [1], we propose the idea that agents, facilitating in the drug delivery, can form stable noncovalent supramolecular or nanobiocomplexes with the drug molecules to be transported through the cell membrane. Based on the mentioned idea the current investigation by electrospray ionization mass spectrometry (ESI MS) is devoted to examining the noncovalent complexes formation between dimethyl sulfoxide (DMSO) known as an agent facilitating the transdermal drug delivery, and a number of antimicrobial drugs: antibiotics chloramphenicol (CAP), levofloxacin (LEF) and antituberculosis agent cycloserine (CYS).

Formation of stable noncovalent complexes of DMSO with the molecules of antibiotics LEF and CYS in the polar solvent methanol has been revealed by ESI MS probing of the double model systems of the DMSO with the drugs with 1:3 molar ratio, on the basis of recording the protonated peaks of $DMSO{\bullet}drug{\bullet}H^+$ complexes in the mass spectra. At the same time the complexation of DMSO with CAP is not revealed in the similar model system DMSO:CAP (1:3 molar ratio). The correlation between the drugs structure features and the noncovalent complexes formation ability with DMSO molecules is discussed.

The results obtained confirm the ESI MS method applicability to study the DMSO complexation with the drugs molecules and biomolecules.

Acknowledgment. Authors acknowledge the Program of cooperation between Ukrainian and Hungarian Academies of Sciences for the financial support of the visits of the scientists from B. Verkin Institute for Low Temperature Physics and Engineering of the NAS of Ukraine to the Research Centre for Natural Sciences in Budapest, where the mass spectrometry experiments were carried out. Grant N 0120U100157 of NAS of Ukraine is appreciated.

[1] V.A. Pashynska, M.V. Kosevich, *Біофізичний вісник*, **2019**, 42, 28-48.

PHOTODYNAMIC THERAPY AS A NEW APPROACH IN THE ACNE VULGARIS TREATMENT

Radko A.S., Melekhovets O.K., Kharchenko T.O., Melekhovets Yu.V.
Sumy State University, 2 Rymskogo-Korsakova st., Sumy 40007, Ukraine
e-mail: radkoalevtina@gmail.com

Introducton. Photodynamic therapy (PDT) is a laser method which use photosensitizer to rich precise tissue target in the inflammation site. Photosensitizer is activated by the light of a certain wavelength. PDT for the treatment of acne is safe, effective, and associated with no or minimal complications, especially when appeared topical photosensitizers.

Aim: to study the efficacy of photodynamic therapy for post-inflammatory treatment in patients with acne vulgaris.

Materials and methods: Total of 90 patients with diagnosis of moderate acne vulgaris, comparable in age and sex, were divided into 2 groups. Patients of the 1st group (n = 40) received basis treatment. The 2nd group (n = 50) patients received PDT course to reduce post-inflammatory changes. The procedure was performed with laser with wavelength - 660 nm. Firstly, chlorine photosensitizer was applied to the affected areas of the skin for 40 minutes in the dark room. Next, laser irradiation was permormed by distans method with 600 mcm optic fibre; the average total dose of energy per procedure 500-700 J (pict.1). The course consisted of 4 procedures, ones a week.

Life quality was determing with using the DLQI questionnaire. Patient’s clinical status was evaluating with the GAGS scale. Examination were performed twice - at the baseline and a month after the therapy.

Results. At the baseline, the GAGS score in the 1st group was 18.2; in the 2nd group - 16.5 points. Results after treatment demonstrated mild improving by 17.1 points in the 1st group, and moderate – by 13.0 points in the 2nd group. The DLQI questionnaire score at the baseline was 4.3 in the 1st group, and 3.75 in the 2nd group. Data dynamic after one-month treatment showed 3.9 points in the 1st group, and 2.75 points in the 2nd group.

Conclusion. It was confirmed, that PDT significantly reduced the post-inflammatory changes following clinical picture improving by 21% and life quality by 40% in patients with acne vulgaris.

Picture 1. PDT procedure in moderate acne vulgaris patient

PONDEROMOTIVE FORCES AS A REASON FOR DESTRUCTION OF VIRUS INTERACTING WITH NANOPARTICLES

V. Lozovski[a], N. Rusinchuk[a], V. Lysenko[b], M. Lokshyn[b], S. Zagorodnya[c], M. Chayka[c], Yu. Mukha[d], N. Vityuk[d]
[a] *Taras Shevchenko National University of Kyiv, 4-g Glushkova ave, Kyiv 03022*
[b] *V. Ye. Lashkaryov Institute of Semiconductor Physics, 45 Nauki ave, Kyiv 03028*
[c] *D. Zabolotny Institute of Microbiology and Virology, 154 Acad. Zabolotnogo str, Kyiv 03680*
[d] *Chuiko Institute of Surface Chemistry, 17 General Naumov str., Kyiv 03164*
e-mail: n.m.rusinchuk@gmail.com

When nanoparticles solution is adding to viruses preparation the nanoparticles may adsorb on the virus surface due to Van der Vaals forces[1]. As a result of such interaction a stable nano-sized system is formed. In such system the local electric field is redistributed by the nanoparticles and viruses, which in turn leads to the local field enhancement effect and appearance of ‘hot spots’ on the virus surface[2]. Consequently, there are local field gradients on the virus surface, and this is the reason for ponderomotive forces acting on the virus. Results of calculations show that on the surface of influenza virus near the Au nanoparticles of 5 nm diameter the forces may lead up to 70 nN. Existed experimental studies indicate that mainly the force higher than 30 nN leads to irreversibile deformation of the virus particle[3]. We suppose that this mechanism (schematically shown in Fig. 1) is the reason of destruction of viruses mixing with nanoparticles, which was demonstrated by microscopy studies for many times.

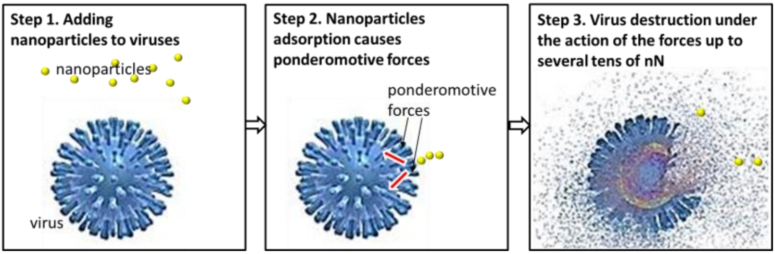


Fig. 1. Scheme of the mechanism of nanoparticles action on the virus

---

[1] V. Lozovski, N. Rusinchuk, T. Vasiliev, *2019 IEEE 39th International Conference on Electronics and Nanotechnology, ELNANO 2019*, 2019, pp. 253-256.

[2] V. Lozovski, V. Lysenko, N. Rusinchuk, *Advances in Natural Sciences: Nanoscience and Nanotechnology*, 2020 In Press.

[3] P.J. de Pablo, M. G. Mateu, *Structure and Physics of Viruses*, 2013, pp. 519-551.

ELABORATION OF NEW APPROACHES FOR PREPARATION OF HIGHLY SENSITIVE CONDUCTOMETRIC BIOSENSORS FOR L-ARGININE DETERMINATION

O.Y. Saiapina[a], S.V. Dzyadevych[a,b]
[a]*Department of Biomolecular Electronics, Institute of Molecular Biology and Genetics of National Academy of Sciences of Ukraine, 150 Academician Zabolotnyi Str., Kyiv, 03680, Ukraine; e-mail: osayapina4@gmail.com*
[b]*Institute of High Technologies, Taras Shevchenko National University of Kyiv, 4H Academician Hlushkov Ave., Kyiv, 03022, Ukraine; e-mail: dzyad@yahoo.com*

Over recent decades, organic and inorganic materials have been widely applied in biosensor technologies due to their potentiality to provide substantial improvements in the analytical performance and impart advantageous functions to the traditional selective materials if used together [1]. Zeolites are among such perspective materials in virtue of their inherent or synthetically derived selectivity to atoms and molecules, enabling their use in (bio)sensors for detection of certain analytes. Clinoptilolite (CLT) belongs to the most abundant family of natural zeolites and is characterized with selectivity to NH_4^+ ions, low cost, and high surface area.

This work presents a novel conductometric biosensor for L-arginine determination based on a natural zeolite clinoptilolite (CLT), directly deposited on the electrode surface, and followed by the enzymatic layer (an arginase-urease membrane cross-linked with glutaraldehyde). In the current work, the effect of co-immobilization of the enzymes and CLT in the layer-by-layer fashion on some analytical characteristics of the L-arginine biosensor was studied. It includes also a comprehensive investigation of the effect of buffer parameters on the biosensor's analytical characteristics. EIS and differential conductometry were used to investigate the sensor performance under varying experimental parameters.

The analysis of the biosensor concentration ranges revealed two adjacent linear regions within a calibration curve (0.1–0.9 mM and 0.9–6.5 mM) that perhaps could be interpreted by the independent impact of the ammonium-exchange properties of the zeolite layer and enzymatic activity of the biomembrane. It was found that in the optimized working buffer (5 mM KH_2PO_4-Na_2HPO_4, pH 7.5) the biosensor had the limit of detection approximately one order of magnitude lower than the biosensor which was not modified with CLT (5.0×10^{-7} M vs. 1.0×10^{-6} M–5.0×10^{-6} M). The CLT-based biosensor had high operational stability; a significant decrease in the operational stability was observed after the 19th day of the biosensor use.

The preliminary studies suggest that the CLT-based conductometric biosensor might be considered as a promising bioanalytical tool for the reliable and affordable L-arginine determination upon the additional investigations with the model samples and eventually – with the real samples.

This work was funded by the grant of National Academy of Sciences of Ukraine for research laboratories/groups of young scientists of NAS of Ukraine for conducting investigations within the priority directions for development of science and technology in 2020.

[1] M. Holzinger, A. le Goff, S. Cosnier. Nanomaterials for biosensing applications: a review. *Front Chem*., **2014**, 2, Article ID 63.

IMPROVING ANTIOXIDANT PROPERTIES OF NANOCERIA BY DOPING AND LASER IRRADIATION

Vladyslav Seminko, Pavel Maksimchuk, Ganna Grygorova, Elena Okrushko, Yuri Malyukin
Institute for Scintillation Materials NAS of Ukraine, 61072, 60 Nauky ave., Kharkiv, Ukraine
e-mail: seminko@isma.kharkov.ua

The ability of cerium oxide nanoparticles (nanoceria) to effective antioxidant defense of the living cells have been discussed in the number of publications since the first observation of their ROS-protective action in 2006, but the mechanism of antioxidant activity of nanoceria and the methods of its improvement still remain unclear. We have revealed that 5d→4f luminescence of Ce^{3+} ions in CeO_{2-x} nanocrystals opens the possibility of controlling the interaction of reactive oxygen species with ceria nanocrystals. Using the methods of optical spectroscopy, we have shown that the antioxidant activity of ceria and ceria-based mixed (CeO_2 - Re_2O_3 (Re = Y, Eu, Tb), CeO_2-ZrO_2) colloidal nanoparticles depends strongly on the temperature, size of nanoparticle, type and concentration of doped ions, and laser irradiation. While for CeO_2-ZrO_2 nanoparticles the rate of H_2O_2 decomposition was higher than in CeO_{2-x} nanoparticles, for other mixed nanocrystals the sufficient slowing-down of H_2O_2 decomposition was observed. This effect was explained by the main role of Ce^{3+}-V_o-Ce^{3+} complexes in the processes of hydrogen peroxide decomposition, which role is similar to the role of active sites of enzymes. The number of Ce^{3+}-V_o-Ce^{3+} complexes increases at Zr^{4+} incorporation due to increase of the content of oxygen vacancies, but decreases at incorporation of isovalent ions (Y^{3+}, Eu^{3+}, Tb^{3+}) leading thereby to higher or lower rate of H_2O_2 decomposition, respectively. On the contrary, for hydroxyl radicals ($^{\cdot}OH$) and superoxide anions (O_2^-) the antiradical activity of ceria nanoparticles is determined not by the content Ce^{3+}-V_o-Ce^{3+} complexes, but merely by Ce^{3+}/Ce^{4+} ratio on the nanoceria surface.

The continuous laser irradiation with specific wavelengths (corresponding to $O^{2-}\rightarrow Ce^{4+}$ charge transfer transitions) leads to formation of additional oxygen vacancies, and so, of additional Ce^{3+}-V_o-Ce^{3+} complexes providing better antioxidant activity of pre-irradiated ceria nanoparticles. Pre-irradiation of nanoceria improves scavenging of different types of ROS including hydrogen peroxide, hydroxyl radicals, and superoxide anions. The same irradiation provides higher rate of recovery of initial antioxidant properties of nanoceria after interaction with reactive oxygen species. So, both doping by different ions and laser irradiation allows to improve antioxidant properties of nanoceria, and opens the way for development of new class of nanomaterials with controlled redox properties for a number of biological and medical applications.

FILM HYDROGELS WITH SILVER NANOPARTICLES FOR THE TREATMENT OF BURNS AND WOUNDS

Volodymyr Skorokhoda, Nataliya Semenyuk, Yuriy Melnyk,
Mykhailo Bratychak, Galyna Dudok
Lviv Polytechnic National University
S. Bandery st., 12, Lviv, 79013, Ukraine
e-mail: vskorohoda@yahoo.com

Film hydrogels are perspective for the making of membranes for medical purposes.

The fundamentals of technologies for the obtaining of hydrogel bactericidal film composite materials based on copolymers of hydroxyalkilmethacrylates with polyvinylpyrrolidone applied for the treatment of wounds and burns have been developed. The basis of mentioned materials are hydrogels, related to biological tissues by physical condition. In order to enhance the mechanical properties, the films have been reinforced during the synthesis with polyamide and polypropylene grid with a cell size of 0.5 ... 2.0 mm. This gave the possibility to increase the tensile strength of the films by 1-2 orders.

The possibility to provide synthesized hydrogel films with anti-thrombogenic properties by immobilization of heparin on its surface was confirmed by the research. The sorption capacity of hydrogels, depending on its composition, can be changed widely ($1\cdot10^4 \ldots 6\cdot10^5$ units/m^2). As it was found the surface heparinization does not reduce the film's permeability for water and low molecular weight substances dissolved in it.

High and adjustable diffusion transport properties of the films make it easy to deliver the medicine to the wound without the coating removing. High optical properties of some copolymers allow them to be applied as antiseptic, therapeutic and corrective contact lenses. The presence of polyvinylpyrrolidone links in hydrogel's composition makes it possible to uniformly form the silver nanoparticles throughout the volume of films. Nanoparticles were obtained from silver salts during the synthesis of hydrogel without the use of toxic restorative reagents. It allowed to provide a film coating with bactericidal properties. In particular, the films demonstrate high and stable fungybactericidal properties relative to E. Coli, S. Aureus and A. Niger.

Medical and biological studies confirm that hydrogel film membranes create an effective barrier against harmful external influences. At the same time, they are elastic, permeable to oxygen and drugs, have good adhesion to the wound without gluing, do not cause allergies. Such film replacing is painless and does not damage the formed early epidermis, along with the film the excretion and dead tissue are removed from the wound. The use of developed silver-containing film membranes accelerates the granulation of the wound surface and prevents its infection.

IMPROVEMENT OF THE METHOD FOR DETERMINING ENERGY CONSUMPTION IN A BIOGAS REACTOR

M.M. Zablodskiy, M.O. Spodoba,
National University of Life and Environmental Sciences of Ukraine, ERI Energetics, Automation and Energy Efficiency, st. Heroes of Defense, 12, 03041, Kiev, Ukraine.
e-mail: spmisha@ukr.net

The profitability of using biogas plants directly depends on the energy efficiency of the methane formation process. Since the energy flow necessary to maintain the level and uniformity of temperature and substrate concentration within the established limits depends on many time-varying factors, determining energy costs is a difficult task. The energy transmitted by mixing and heating devices requires a certain amount of electrical energy and carrying out an accurate analysis of energy costs and optimization of this process.

To determine the energy costs, a comprehensive mathematical model is proposed that takes into account the interconnected processes of converting electrical energy into thermal and mechanical, the equations of motion of the substrate, the energy costs associated with the electric drive and electric heaters, the heat costs of heating the substrate in a biogas reactor.

The basis for determining the heat loss to maintain a constant temperature of anaerobic fermentation is the heat balance equation. With the well-known definition of components, the heat balance equation takes into account the heat of the existing substrate in the bioreactor (Q_{sub}), heat of fermentation (Q_f), heat of the heating device (Q_{heat}), heat loss to the environment (Q_{en}), with allotted biogas (Q_b), and spent substrate (Q_s). The difference between the method is to take into account the dynamics of mixing the substrate and the influence of the thermal energy of the fresh substrate $(Q_{fr.sub})$, which is loaded into the reactor.

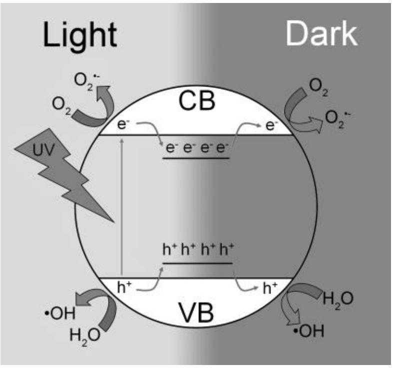
Based on the results of a numerical experiment according to the proposed model, the flow distributions and patterns of energy conversion are determined, and new technical solutions are formed to increase the energy efficiency of biogas plants.

MULTIFUNCTIONAL $ReVO_4:Eu^{3+}$ NANOPARTICLES IN THERANOSTICS

S.L. Yefimova[a], P.O. Maksimchuk, K.O. Hubenko, V.K. Klochkov, Yu.V. Malyukin
Institute for Scintillation Materials NAS of Ukraine, 60 Nauky Ave., Kharkiv 61072, Ukraine)
e-mail: ephimovasveta@gmail.com

Theranostics is a new pioneering approach in modern biomedical researches. This approach allows combination of both therapeutic (drugs) and diagnostic or other agents (fluorescent molecules or nanoparticles, iron oxide nanoparticles, *etc.*) in a novel therapeutic formulation. The field of “theranostic nanoparticles” aims to use unique properties and physical characteristics of nanomaterials for the diagnosis and treatment of diseases at the molecular level. For example, in cancer nanotheranostics, nanoparticles are functionalized by combining imaging and therapeutic agents to interact with cancer cells at the molecular level in such a way that the functionalized combo particles can significantly improve the effectiveness and specificity of therapy to cancers that are currently difficult to treat.

Despite the fact that the number of publications and launched clinical trials investigating nanomedicine drugs for cancer therapy increase constantly over the last 10 years, the total number of clinical trials is only about 2% of the total number of publications in the field of cancer nanomedicine. The next step in theranostic medicine is the applications of nanoparticles (NPs) with multiple functions that allows multimodal therapy to be realized. Multifunctional nanoparticles are able to carry out two or more functions simultaneously, such as imaging and treatment of the target disease.



In this study, we report on multifunctional $ReVO_4:Eu^{3+}$ NPs, which possess luminescent, scintillation and triggered redox properties that allows them to be considered as theranostics agents. It was revealed that depending on pre-treatment conditions, the same $ReVO_4:Eu^{3+}$ NPs could act as pro- or anti-oxidant. Redox properties of $ReVO_4:Eu^{3+}$ NPs have been studied in water solutions and biological environment (lipid suspension, cells) and *in vivo* experiments. It was shown that redox-activity of $ReVO_4:Eu^{3+}$ NPs are responsible for their anti-tumor action, wound healing effect, radioprotective and anti-aging effects that opens new way for this nanomaterial applications in biomedical area.

Scintillation properties of $ReVO_4:Eu^{3+}$ NPs allow them to be considered as “light source” for photo-sensibilizator molecules in such a method of cancel treatment as X-ray excited photodynamic therapy.

DETERMINATION OF OPTIMUM APEX ANGLE OF CONE-SHAPED PART OF PELLETIZER DIE BY MEANS OF SIMULATING BIOMASS GRANULATION PROCESS

[1]Polishchuk Viktor, [1]Tarasenko Svitlana, [1]Antypov Ievgen , [2]Bilyk Stepaniia
[1]*National University of Life and Environmental Sciences of Ukraine*
15, Heroyiv Oborony Str., Kyiv, 03041, Ukraine
e-mail: polischuk.v.m@gmail.com
[2]*Separated Subdivision of National University of Life and Environmental Sciences of Ukraine "Berezhany Agrotechnical Institute"*
20, Akademichna St., Berezhany, Ternopil region, 47501, Ukraine

The key disadvantage of granulated biofuel is high energy costs of its production. The costs can be reduced by optimizing matrix design and process parameters including the measure of the apex angle of the cone-shaped part of a matrix die. Literature data analysis did not make it possible to determine the optimum measure of the apex angle of a cone-shaped die part under the condition of minimum energy cost of the pelletizing process.

Thus, the research is aimed at determining the optimum apex angle of the cone-shaped part of a granulator die under the condition of minimum energy cost of the pelletizing process by means of simulating the process of biomass granulation.

The dependence $P_{pr} = f(2\gamma)$ was determined by means of simulating the process of biomass granulation; it was tested for the extremum $P_{pr} \rightarrow \min$ using dichotomy method. Functional dependence of the apex angle of the cone-shaped part of a pelletizer die on the height of a raw material layer, which is taken in by a roller during pressing has been determined. Under the condition of pressure reduction, the optimum apex angle of the cone-shaped part of a granulator die is equal to 26° at h_{pr} = 1 mm, 32° at h_{pr} = 2 mm, 41° at h_{pr} = 3 mm, 59° at h_{pr} = 4 mm, 109° at h_{pr} = 5 mm, 122° at h_{pr} = 6 mm, 131° at h_{pr} = 7 mm and it is approximated with the accepted coefficient of determination by Newton quartic polynomial, which makes it possible to determine the design and process parameters of a granulation unit under the condition of minimum energy costs of pressing [1].

Reference

1. Polishchuk, V.M. (2019). Theoretical and experimental justification of technical and technological system of production and use of biofuels in agriculture. Extended abstract of doctor's thesis. Kyiv: NUBiP of Ukraine [in Ukrainian].

SECTION 8

PHYSICS AND TECHNOLOGY OF ORGANIC SOLAR CELLS, LEDS, FETS, SENSORS, CONJUGATED THIN FILMS FOR ELECTROCHROMIC DEVICES.

SYNTHESIS AND CHARACTERIZATION OF ELECTROACTIVE MATERIALS FOR AIEE PROPERTIES

Ronit Sebastine Bernard[a], Galyna Sych, Sohrab Nasiri, Oleksandr Bezvikonnyi, Dmytro Volyniuk, Azhar Ariffin, Viktorija Andrulevicienė, Juozas V. Grazulevicius
[a]*Department of Polymer Chemistry and Technology, Kaunas University of Technology, Radvilenu pl. 19, LT-50254, Kaunas, Lithuania.* ronit.bernard@ktu.edu

Triphenylethylene (TPE) based derivatives are used to achieve aggregation induced enhanced emission (AIEE) in order to solve the problem of aggregation caused quenching (ACQ) [1]. Materials with TPE units can provide high emission efficiencies in the aggregated state that can be effectively used to fabricate efficient non-doped OLEDs [2]. The synthesized compounds were based on a donor acceptor rotor (D-A-R) molecular structure where TPE unit was used as rotor. D-A-R materials demonstrate AIEE and bipolar properties [3]. Photoluminescence decay was measured to study the fluorescence time and prompt fluorescence was observed without the delayed fluorescence, leading to the AIEE properties measurement by the mixture of THF/H_2O solution, as the H_2O concentration got increased a drastic elevation in the intensity of materials was observed proving the AIEE behaviour (Fig. 1). The best non-doped device fabricated based on the synthesized D-A-R material showed turn-on voltage of 4.2v, maximum brightness of 5700 cd/m2 and power efficiency of 3.2 lm/W.

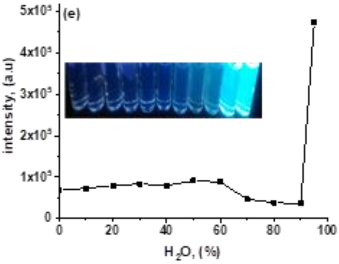


Fig. 1. PL intensity of compound in the THF/Water mixtures

Acknowledgement: This work was supported by the Research Council of Lithuania (Grant No **S-LU-20-12**).

[1] H-T. Lin, C-L. Huang and G-S. Liou, *ACS Appl. Mater. Interfaces*, **2019**, 11, 11684.
[2] J. Guo, X-L. Li, H. Nie, W. Luo, S. Gan, S. Hu, R. Hu, A. Qin, Z. Zhao, S-J. Su and B. Z. Tan, *Adv. Funct. Mater.*, **2017**, 27, 1606458.
[3] G. Sych, J. Simokaitiene, O. Bezvikonnyi, U. Tsiko, D. Volyniuk, D. Gudeika and J. V. Grazulevicius, *J. Phys. Chem. C*, **2018**, 122, 14827.

ELECTROOPTICAL TRANSITIONS IN CONJUGATED POLYMER SYSTEMS

Aksimentyeva O.I.

Ivan Franko National University of Lviv, 6 Kirila-Mefodia, 79005, Lviv, Ukraine
aksimen@ukr.net

Conducting polymer systems present electron delocalization, arising from conjugated double bonds in the polymer backbone. They show an electrical conductivity in doped states (*p*-doping or *n*-doping) and are insulators when they are undoped (neutral state). As a result of electrochemical doping-dedoping processes, the electronic properties (e.g. band gap) of the conjugated polymer can be essentially varied [1,2]. This correspond to modified optical properties (e.g. absorption bands) and is relate with color changes. It is believed that electrooptic phenomena are determined by both energetic properties of organic molecules in the ground and excited states and the factors characterized the transition from one state to another. Change of color is associated with the injection or extraction of charge, which accompanies the oxidation - reduction processes in the polymer chains. After the discovery of electrochromic effect, many inorganic and polymeric materials have been used for industrial applications, including for "smart" windows, car mirrors, non-emitting flat organic displays, infrared sensors, etc. These devices are soft to the human eye, do not emit electromagnetic and ionizing radiation.

This report presents the new approaches to obtain the multicolor and hybrid films based on conducting polymers and composites as well as the interconnection of electronic transitions with electrochemical and optical response in conjugated systems. The proposed electro-optical elements with electrochromic polymer layers are characterized by optical memory, low cost and easy of application technology of polymer layer, that makes them preferable to liquid crystal displays. The novelty of this development lies in using the electrochromic layers of conjugated polymers with electron and ionic conductivity obtained on the transparent electrodes by the method of electrochemical polymerization [1].

Our investigation is directed on the synthesis and study the electrochromic hybrid layers of conducting polymers (poly-3,4-ethylenedioxytiophene, polyaniline, polyanisidine and polyindole) with semiconductor or carbon nanoparticles (porous silicon [3], TiO_2, graphene oxide, etc.). We developéd the methods to obtaining hybrid systems based on conducting polymers incorporated into dielectric polymer matrices [4] and study their structure, optical, electrical and electrochemical properties. On the base of obtained results, the new methods to producing flexible optical elements of organic electronics are proposed.

[1]. O. I. Aksimentyeva, O. I. Konopelnyk, D.O. Poliovyi, *Computational and experimental analysis of functional materials*. Toronto: Apple Academic Press, **2017,** 91–150.
[2]. T.-H. Le, Y. Kim, H. Yoon, *Polymers,* **2017,** 9, 150; doi:10.3390/polym9040150
[3]. I.B. Olenych, O.I. Аксіментьєва, L.S. Monastyrskii. Patent № 127257 (UA). **2018**, Bul. № 14.
[4]. Yu. Bashtyk, I. Kremer, A. Fechan, O. Aksimentyeva, Yu. Horbenko, et al., *Mol. Cryst. Liq. Cryst.* **2018**. 672 (1), 150–158. –**doi:** 10.1080/15421406.2018.1550546.

DERIVATIVES OF TRIAZINE AND *TERT*-BUTYLCARBAZOLE AS TADF EMITTERS FOR OLEDS

Oleksandr Bezvikonnyi[a], Dalius Gudeika[a], Dmytro Volyniuk[a], Juozas V. Grazulevicius[a]
[a]*Department of Polymer Chemistry and Technology, Faculty of Chemical Technology, Kaunas University of Technology, Radvilenu pl. 19, LT-50254, Kaunas, Lithuania*
e-mail: juozas.grazulevicius@ktu.lt

Organic light emitting diodes (OLEDs) took a lead in the industry of lighting and display devices. Efforts are required to maintain the dominance by solving of the problem of low efficiency of emission of blue light. The approach of thermally activated delayed fluorescence (TADF) was reported as a method to increase the internal quantum efficiency of emitters by four times comparing to ordinary fluorescent emitters [1]. With suitable molecular geometry, thermal motion of atoms results in a reverse intersystem crossing of triplet excitons to the first excited singlet state. The strong donor-acceptor character of π-conjugated system leads to a minimization of splitting between energy levels of the first singlet and triplet excited states. Carbazole as a donor moiety with high triplet energy is widely used as a donor moiety in the design of TADF compounds [1]. *Tert*-butyl substitution can block the non-radiative pathways of excitation energy deactivation for facilitating TADF. Triazine accepting moieties are also often used in structures of TADF emitters [1]. Here, we present properties of the series of derivatives of triazine and *tert*-butyl carbazole.

The studied sky-blue emitters have a singlet-triplet energy splitting less than 0.1 eV. Bathochromic shift of the emission peak of dilute solutions with the change of solvent to more polar discloses intramolecular charge transfer character of the luminescence. For the fabrication of OLEDs exhibiting TADF, guest:host systems based on hole-transporting 1,3-bis(N-carbazolyl)benzene (mCP) host were investigated. The doped films exhibited photoluminescence quantum yield values in the range of 32-64%. Prompt and delayed fluorescence owed the same spectral profile pointing to the triplet harvesting through the mechanism of reverse intersystem crossing. Thermal activation of the delayed fluorescence at ~180 K was manifested from the analysis of emission decay curves recorded in inert atmosphere. Employment of these guest:mCP systems as emitting layers of OLEDs led to obtainment of maximum current efficiency up to 15 cd/A with the wavelength of electroluminescence peak around 475 nm.

Acknowledgment. This project has received funding from the Research Council of Lithuania (LMTLT), agreement No [S-LU-20-3].

[1] Y. Tao, K. Yuan, T. Chen, P. Xu, H. Li, R. Chen, C. Zheng, L. Zhang, W. Huang. *Adv Mater.*, **2014**, 26(47), 7931-7958.

THE INFLUENCE OF MgO ADDITION ON RED PHOTOLUMINESCENCE OF Mn^{4+} ACTIVATED Zn_2TiO_4 PHOSPHORS

L. Borkovska[a], T. Stara[a], I. Vorona[a], V.Nosenko[a], K.Kozoriz[a], C. Labbé[b], J. Cardin[b], J.-L. Doualan[b]

[a] *V. Lashkaryov Institute of Semiconductor Physics of NAS of Ukraine, 45 Pr. Nauky, Kyiv 03028, Ukraine*

e-mail: l_borkovska@ukr.net

[b] *CIMAP, UMR 6252, CEA-CNRS-ENSICAEN, Normandie Université, 6 Blvd Maréchal Juin, 14050 Caen, France*

Recently, Mn^{4+}-activated inorganic luminescent materials have attracted much interest for application in phosphor-converted white light-emitting diodes (LEDs) as the cost-effective alternatives to rare-earth doped red phosphors. Titanates are considered as the proper hosts for Mn^{4+} ions because substitution of Ti^{4+} by Mn^{4+} does not need charge compensation. Besides, titanates are distinguished by excellent thermal stability and environmental safety. However, quantum efficiency of Mn^{4+} emission in titanates is limited by PL thermal quenching and incorporation of manganese in +2 charge state.

In this work, the influence of addition of excess MgO (10, 30 and 60wt%) on red PL of Mn^{4+} activated Zn_2TiO_4 phosphors has been investigated by PL and electron paramagnetic resonance (EPR) methods. The phosphors were produced by solid-state reaction via sintering in air at 1050, 1100 and 1150°C of a mixture of ZnO, MgO and TiO_2 powders. An aqueous $MnSO_4$ solution was added to powder mixture to provide Mn content of about 0.1 mol %.

The Mn doped Zn_2TiO_4 phosphors demonstrated PL band peaked at about 680 nm due to $^2E_g \rightarrow {}^4A_{2g}$ spin forbidden transition of Mn^{4+} ions in Zn_2TiO_4 crystal lattice. The PL intensity was rather low apparently because of intense thermal quenching. In fact, at liquid nitrogen temperature the PL intensity increased more than ten times. This conclusion was proved by relatively short PL relaxation times of about 100 μs. The EPR spectra of Mn doped Zn_2TiO_4 phosphors did not show the signal caused by Mn^{2+} ions.

The phosphors produced with an excess MgO showed strongly increased red PL peaked at 670 nm. The shift of PL band maximum to shorter wavelengths indicated formation of $(Zn_xMg_{1-x})_2TiO_4$ solid solution. The PL relaxation time increased up to 450 μs that evidenced to the decrease of PL thermal quenching. The EPR spectra of the phosphors with 10 wt% excess MgO revealed a signal due to Mn^{2+} ions in $(Zn_xMg_{1-x})_2TiO_4$ crystal lattice. However, adding of 30 and 60wt% excess MgO completely suppressed formation of Mn^{2+} centers in $(Zn_xMg_{1-x})_2TiO_4$ matrix. This agreed with higher intensity of Mn^{4+} red PL in the phosphors with 30wt% excess MgO as compared with those with 10wt%. The largest increase of PL intensity about 36 times was found in the phosphors with 30wt% excess MgO sintered at 1050 °C. It is concluded that adding of an excess MgO is an efficient tool in increasing the efficiency of red phosphors based on Mn^{4+} activated zinc magnesium titanates.

ORGANIC-INORGANIC NANOSTRUCTURED SENSING MATERIALS WITH TUNABLE ADSORPTION PROPERTIES

J. Burlachenko[a], I. Kruglenko[a], B.Snopok[a]
[a] *Institute of Semiconductor Physics NAS of Ukraine, Nauki av. 4, Kyiv 03028 Ukraine*
e-mail: julia.burlachenko@gmail.com

Hybrid nanostructures based on a combination of components of various nature open up the possibility of creating new materials with the advanced properties tuned for specific applications. In this work, organic-inorganic nanostructured layers were developed and tested as sensing elements with tunable adsorption properties.

Nanostructured sandwich-like film based on ZnO nanoparticles and a phthalocyanine was used as a sensitive layer for quartz crystal microbalance (QCM) chemical gas sensors. The sensor was illuminated by LEDs with wavelengths of 472 and 615 nm. It was shown that the sensitive film changes its adsorption properties towards alcohols under illumination[1] due to changes of the electronic structure of film's molecules inducing variation of chemical reactivity. A three-sensor array was developed with one real sensor and two virtual ones operating under illumination. This approach allowed us to discriminate three alcohols with the only one sensor. Ethanol, methanol and isopropanol have quite similar physico-chemical properties they have radically different biological impact. In such a way alcohols are interesting test analytes and their discrimination is an important practical task. The results of effective classification by cluster analysis in fuzzy logic format are shown on Fig.1.

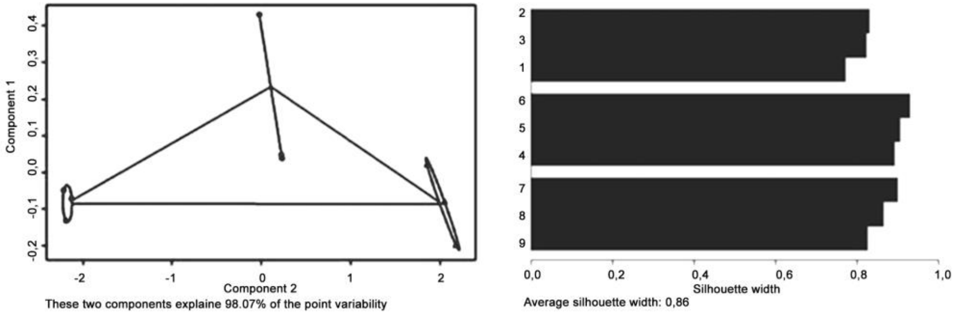


Figure 1 – The results of cluster analysis of three alcohols: ethanol (1,2,3), methanol (4,5,6) and isopropanol (7,8,9) by virtual sensor array based on one QCM sensor with ZnO-copper phthalocyanine sensitive layer without illumination and under illumination by 472 and 615 nm.

1.Yu. V. Burlachenko, B. A. Snopok, "Multisensor arrays for gas analysis based on photosensitive organic materials: An increase in the discriminating capacity under selective illumination conditions", Journal of Analytical Chemistry, **2008,** 63 (6), pp. 557–565.

STRUCTURE, OPTICAL AND SENSORY PROPERTIES OF POLY-3,4-ETHYLENEDIOXYTHIOPHENE FILMS DOPED WITH GRAPHENE OXIDE

Horbenko Yu. Yu.[a], Glazunova V. A.[b], Ivaniuk H. B.[c], Matkivska G. M.[a], Vistak M.[d],
Starykov G. O.[a], Aksimentyeva O. I.[a]
[a] *Ivan Franko National University of Lviv, 6/8 Kyryla&Mefodia st., Lviv 79005, Ukraine*
[b] *O.Galkin Donetsk Institute for Physics and Engineering, 46 Nauky ave., Kyiv 03680, Ukraine*
[c.] *Lviv Polytechnic National University, 12 Bandera st., Lviv 79013, Ukraine*
[d] *Danylo Halytsky Lviv National Medical University, 69 Pekarska st., Lviv 79010, Ukraine*
e-mail: y_bilka@ukr.net

Poly-3,4-ethylenedioxythiophene (PEDOT) has been extensively researched in electrochemical fields owing to its unique structure, high conductivity, environmental and electrochemical stability, superior transparency in the doped state. The PEDOT-based composites with inorganic nanoparticles obtain improved performances like large surface area and fast electron transfer due to the synergistic effects from the individuals.

The conditions of electrodeposition of the PEDOT on the surface of a semiconductor optical transparent SnO_2 electrode under cyclic potential sweep mode have been established. Due electron microscopy synthesized polymer films have a globular structure with uniform distribution by size of aggregates of 80-90 nm. It has been found that doping with graphene oxide nanoparticles (GO) leads to increasing of globule sizes to 200-250 nm and formation of layered structure with graphene plates.

Also, it causes a change in the electronic structure of the polymer – increasing the length of conjugation and concentration of charge carriers and acts as an acceptor dopant. The influence of the electric field on the optical properties of PEDOT and PEDOT/GO films was studied. Electrochromic transitions were observed– the change in the position and intensity of the absorption maxima and, accordingly, the color of films under the action of the applied potential. Using the CVA method, the parameters of charge transport in both PEDOT and PEDOT/GO films were determined. Effective diffusion coefficients were D_{ef} = $(7,82\pm0,07)\times10^{-10}$ cm^2/s for PEDOT and $(9,48 \pm 0,07)\times10^{-10}$ cm^2/s for PEDOT/GO. It has been revealed that doping with GO reduced the diffusion transition time for the PEDOT from 0.29 to 0.23 s, which confirms the improvement of the quick-action of electrochromic films.

It was found that films based on PEDOT can be used to detection toxic gases (NO_2, H_2S) and organic solvent vapors. Isosbestic points on the spectral dependencies of the optical absorption suggest the possibility of selective detection of dimethylformamide with the use of PEDOT as a sensitive element of optical sensors. By electron microscopy is shown that gas action changes morphology of the films. Besides, it was established that doping of PEDOT with graphene oxide significantly increased (by 10 times) the sensory sensitivity of the obtained films to nitrogen (IV) oxide.

GREEN PHOTOLUMINESCENCE OF N-ANNELATED PERYLENES IN A DISTRIBUTED FEEDBACK CAVITY.

I.Dupliak [a], A. Bucinskas[c], Kh. Ivaniuk[b], H. Petrovska[b], D. Volyniuk[c], V. Fitio[b], P.Stakhira[b], J. V. Grazulevicius[c]

[a] Wenzhou University Institute of Laser and Optoelectronic Intelligent Manufacturing Ocean Science and Technology Innovation Park, No. 19 Binhai 3rd Road, Yongxing Street, Longwan District, Wenzhou, Zhejiang, China

[b] Lviv Polytechnic National University, S. Bandera 12, 79013 Lviv, Ukraine

[c]Department of Polymer Chemistry and Technology, Kaunas University of Technology, Radvilenu Plentas 19, LT-50254 Kaunas, Lithuania.

e-mail: khrystyna.b.ivaniuk@lpnu.ua, tel.: +380636072294

For organic lasers, one very important task is to match the luminescence properties of the organic emitters (gain medium) to the optical design of the cavity used. Here, the emission wavelength needs to be compatible with the stop-band of a vertical cavity structure and the designed optical mode. One design that can meet industrial demands is the distributed feedback (DFB) cavity [1].

The generation wavelength is associated with a lattice period and a steady propagation in a planar waveguide, where the active medium has a maximum refractive index. It is most rational to manufacture such lasers under the second-order Bragg conditions. In this case, the direction of propagation of the generated radiation is almost perpendicular to the plane of the waveguide, and the generation wavelength is determined by the expression $2\pi/\Lambda = \beta(\lambda)$, where Λ is the lattice period, β is the propagation wave, and λ is the generation wavelength [2]. Embossed gratings for such lasers can be manufactured using standard technology of rainbow holograms,and the production of such lasers can be quite cheap.

In this work, we realized for the first time N-annelated perylenes DFB cavity by nanoimprinting a corrugated structure onto organic semiconductor template, followed by the subsequent evaporation of a conformal organic layer. More specifically, we manufacture corrugated N-annelated perylenes films with periodicities from 370-440 nm by nanoimprinting a UV-curable polymer resist, coated on a pre-clened glass substrate. Then, the textured N-annelated perylenes films get evaporated thermo-vacuum technic by a film of ~ 400-nm thick organic semiconductor. The photoluminescence quantum efficiency of these solidstate film was determined to be ~42 %.

[1] Y. Yao, X. Chen, Y. Dai, and S. Xie *IEEE Photon. Technol. Lett.*, 2006, vol. 18, no. 1, pp. 187–189.

[2]T.N. Smirnova , O.V. Sakhno, J. Stumpe, and V.M. Fitio, *JOSA B.*, **2016**, V. 33, No 2, pp. 202 – 210.

NEW MECHANISM OF THERMAL CONDUCTIVITY OF MOLECULAR SUBSTANCE

A. I. Krivchikov[a], O. A. Korolyuk[a], O. O. Romantsova[a], Yu. V. Horbatenko[a],
A. Jeżowski[b], D. Szewczyk[b]
[a] *B.Verkin Institute for Low Temperature Physics and Engineering of the NAS of Ukraine, 47 Nauky Ave., Kharkiv, 61103, Ukraine*
[b] *Institute of Low Temperature and Structure Research, PAS,*
2 Okólna Str., 50-422, Wrocław, Poland
e-mail: krivchikov@ilt.kharkov.ua

Many efforts are being made to find new perspective irregular solids (glasses, amorphous, etc.), complex crystals, and meta-materials with controlled thermal properties.

The temperature dependence of thermal conductivity κ(T) of selected molecular polycrystals consisting of flexible molecules was investigated within 20–260 K. The materials were para-chloronitrobenzene, penta-chloronitrobenzene and freons F-112 and F-113 [1]. The κ(T) of these crystals increased with temperature in the interval where processes of phonon–phonon scattering were dominant. The increase was observed both in the orientationally-ordered and -disordered phases and is typical of the thermally activated heat transfer by localized molecular excitations. The experimental facts indicate to the presence in the investigated solids of new thermal conductivity mechanism of thermoactivation type, which uniquely reflects one of the new key points, namely - heat transfer by jumps of intramolecular high-energy excitations above cryogenic temperatures [2]. The results are relevant to both fundamental science and practical terms, as they open the way to the design of new functional materials whose properties are governed by optical methods, and the creation of thermal nano-valves and diodes based on them.

[1] Yu. V. Horbatenko et al. *Journal of Phys. and Chem. of Solids*, **2019**, 127, 151–157.

[2] M.A. Strzhemechny et al. *Chem. Phys. Lett.*, **2016**, 647, 55–58.

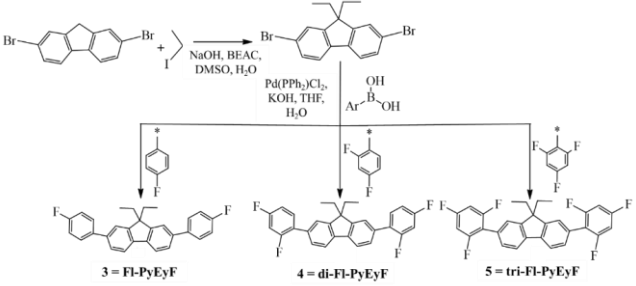
NEW STRUCTURE HOLE TRANSPORTING DERIVATIVES FOR PHOSPHORESCENT OLED DEVICES

Gintare Krucaite,[b] Deepak Kumar Dubey,[a] Sujith Sudheendran Swayamprabha,[a] Rohit Ashok Kumar Yadav,[a] Dovydas Blazevicius,[b] Jairam Tagare,[c] Sudam Chavhan,[a] Tsung-Chia Hsueh,[a] Sivakumar Vaidyanathan,[c] Saulius Grigalevicius,[b] Jwo-Huei Jou[a]

[a]*Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu, 30013, Taiwan*
[b]*Department of Polymer Chemistry and Technology, Kaunas University of Technology, Radvilenu plentas 19, LT50254, Kaunas, Lithuania*
[c]*Department of Chemistry, National Institute of Technology Rourkela, India*
e-mail: gintare.krucaite@ktu.lt

OLEDs bring the several unique benefits, such as superior image quality, ease of fabrication, conformability to curved structures, low power consumption, high-speed video rate, low-cost, wide viewing angle, wide color gamut, mechanical robustness, surface emission, and transparency [1-2].

The synthesis of dual fluorophenyl, difluorophenyl or trifluorophenyl substituted 2,7-diaryl 9,9-diethylfluorenes derivatives, Fl-PyEyF, di-Fl-PyEyF and tri-Fl-PyEyF was carried out by a multi-step synthetic route as shown in Scheme 1.



Scheme 1.

All the molecules exhibited high thermal stability, high triplet energy, outstanding solubility in common organic green solvents, appropriate molecular orbital energy level, and suitable ionization potential to work as a hole transporting layer in OLEDs. The tri-Fl-PyEyF based yellow phosphorescent OLED device revealed a maximum PE of 39.5 lm/W and CE of 61.0 cd/A, that improves by 55.8 and 52.8%, respectively, compared to the NPB based control OLED device.

Reference:
[1] Z. Wu and D. Ma. *Materials Science and Engineering R: Reports*. **2016**, 107, 1–42.
[2] S. R. Forrest, M. E. Thompson. *Organic Electronics and Optoelectronics, Chem. Rev*. **2007**, 107, 923–925.

Acknowledgments. This research was funded by grant 106-2119-M-007-011- from Ministry of Science and Technology of Taiwan and by a grant No. S-LLT-19-2 from the Research Council of Lithuania.

THE INFLUENCE OF PHOSPHORUS AND CHLORINE ORGANIC VOLATILE COMPOUNDS ON THE SENSOR PROPERTIES OF ELECTROCONDUCTIVE COMPOSITE FILMS

Kukla O.L.[a], Mamykin A.V.[a], Pud A.A.[b], Ogurtsov N.A.[b]
[a] *V.E. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine*
41, Nauki prosp., Kyiv, 03028, Ukraine, e-mail: kukla@isp.kiev.ua
[b] *V.P. Kukhar Institute of Bioorganic Chemistry and Petrochemistry, NAS of Ukraine*
50, Kharkivske shose, Kyiv, 02160, Ukraine, e-mail: alexander.pud@gmail.com

The effect of vapor of phosphorus and chlorine organic volatile compounds on the conductivity of composite chemoresistive films based on electrically conductive polymer of poly-3-methylthiophene doped with chlorine (P3MT-Cl) with polymeric nanoparticles (ball-shaped particles of polyvinylidene fluoride) and carbon nanotubes have been investigated [1]. The range of sensitivity to these analytes was in the range of 10-1000 ppm. The analyte influence on the conductivity of the films consist in the increase the conductivity under the action of chlorine compounds and the reduction the conductivity under the action of phosphorus compounds. It is shown that to ensure the reproducibility of the magnitudes of the responses, before measurements it is necessary to hold the chemoresistive films in analyte vapor of the maximum concentrations used (500-1000 ppm) for 10-20 min. Four types of films were selected for sensor analysis. The statistics of the film responses allowed us to estimate the error of measurement of the particular analyte concentration: from 20 to 40% at maximum concentrations, and at low concentrations (100-200 ppm) the error was significantly increased due to the drift of the baseline of the sensors.

To increase the sensitivity of the chemosensors used, the optimal conditions for the formation of P3MT composite films were determined, as well as optimal ratios in the films composition of electroconducting polymer and nanoparticles of different types. For films with carbon nanoparticles, the optimal composition ratio was 50:50 and 60:40, for films with polymeric nanoparticles it's 90:10. It was shown that for a pure P3MT-Cl film, the maximum response was about 1% (for 1000 ppm of dimethylmethyl phosphonate), while for the above optimal composition of carbon and polymer nanoparticles, the maximum responses were 2% and 7%, respectively for the same vapor concentration.

The optimal variants of the composition of the sensor array, suitable for the identification of vapors of phosphorus and chlorine organic volatile compounds, have been determined. It is shown that only 2-3 types of selected films are sufficient for reliable identification.

[1] Ogurtsov N., Bliznyuk V., Mamykin A., Kukla O., Piryatinski Yu., Pud A. Poly(vinylidene fluoride)/poly(3-methylthiophene) core-shell nanocomposites with improved structural and electronic properties of the conducting polymer component, *Physical Chemistry Chemical Physics journal*, **2018**, Vol. 20, pp. 6450-6461.

SOLUTION-PROCESSED WHITE ORGANIC LIGHT-EMITTING DIODE BASED ON TWO EMISSIVE LAYERS

Malek Mahmoudi, Jonas Keruckas, Dmytro Volniuk, Jurate[a] Simokaitiene[a], Juozas V.Grazulevicius
Department of Polymer Chemistry and Technology, Kaunas University of Technology,
Radvilenu pl. 19, LT-50254, Kaunas, Lithuania
e-mail: malek.mahmoudi@ktu.edu

White organic light-emitting diodes (WOLEDs) are targeted towards display applications for use mainly as liquid-crystal display backlights. There is still a huge potential to investigate solution-processed WOLEDs on account of their very low cost production and suitability for commercially energy-saving large-area panels [1]. The advancement in new efficient organic electroactive materials and relevant knowledge on the structure-properties relationship of the materials can ensure further innovative achievements in the field of OLED technologies.

In this work, novel bicarbazole-based compounds (named JK85 and JK89) with hole mobilities achieving of 4.1×10^{-4} $cm^2V^{-1}s^{-1}$ at high electric fields were selected for WOLED fabrication. Green exciplex-based thermally activated delay fluorescence (TADF) with maxima at 521nm and 519nm were identified for solid-state mixtures JK85:PO-T2T and JK89:PO-T2T based on the selected compounds and conventional exiplex-forming acceptor 2,4,6-tris[3-(diphenylphosphinyl)phenyl]-1,3,5-triazine (PO-T2T), respectively. White electroluminescence was obtained using blue fluorescent TFB, green TADF exiplex-based JK89:PO-T2T, and red phosphorescence $Ir(piq)_2(acac)$ emitters in a device structure ITO/MoO_3(1nm)/TFB:$Ir(piq)_2(acac)$(5 wt%, 30 nm)/ JK85:PO-T2T or JK89:PO-T2T (1x1) (20 nm)/ TSPO1(8 nm)/TPBi(40 nm)/LiF:Al. As a result, the fabricated devices were characterized by high-quality of white electroluminescence with CIE1931 coordinates of (0.384, 0.399) and (0.396, 0.452), recpectivly. The best device showed maximum luminance of 8980 cd m^{-2}, current efficiency of 11.6 cd/A, power efficiency of 5.4 lm/W and external quantum efficiency of 6.2%.

Acknowledgements. This work was supported by the Research Council of Lithuania within scientific co-operation program between Lithuania and Ukraine ("LUW", S-LU-20-9).

[1] S. Wang, L. Zhao, B. Zhang, J. Ding, Z. Xie, L. Wang, W.Wong, *ISience.*, **2018**, 6, 128-137

POLYMER ELECTROLYTE MEMBRANES BASED ON PEO-CONTAINING BLOCK COPOLYMERS

Larisa Kunitskaya, Tatyana Zheltonozhskaya, Stanislav Nessin, Valeriy Klepko
Institute of Macromolecular Chemistry NAS of Ukraine, 48 Kharkovskoye Shosse, 02160 Kiev, Ukraine
e-mail: larisa_kunitskaya@ukr.net

During the last decade solid polymer electrolytes (SPEs) have attracted increasing attention due to their possible application in most energy storage/conversion devices, particularly Li-ion batteries (LBs), dye-sensitized solar cells (DSSCs), fuel cells (PEFCs), etc. For these devices a non-corrosive, high conductive, electrochemically and chemically stable, low cost electrolyte is very important. The solid solvent-free polymer electrolyte based on amorphous polymer materials could be the best for these purposes.

Among the available polymer matrix of the SPEs, poly(ethylene oxide), PEO, and its derivatives are the most widely studied because they have flexible macromolecular backbone which enables ionic transport, superior electrochemical stability to lithium metal, low glass transition temperature (T_g), excellent solubility to conductive lithium salts and good interface stability against Li anode. However, the high crystallinity of PEO leads to low ion conductivity and inferior Li^+ transference numbers (0.2–0.3) at room temperature, which affects the high rate capability of LBs.

In the present work, we investigated triblock copolymers comprising chemically complementary poly(ethylene oxide)/polyacrylamide ($TBC_{PEO/PAAm}$) and their partially hydrolyzed derivative ($TBC_{PEO/P(AAm-co-AAc)}$) as possible ion-conducting membranes for LBs, DSSC and PEFCs.

Two triblock copolymer samples consisting of PEO blocks with variable block length (M_nPEO=$6 \cdot 10^4$ and $3.5 \cdot 10^4$ kDa) and their partially hydrolyzed derivative were synthesized and used for this purpose.

The molecular parameters of obtained TBC are determined by the ^{1}H NMR spectroscopy. Measurement of dielectric characteristics of the studied systems was performed in the frequency range 10^2-10^5 Hz using a dielectric spectroscope developed on the basis of the AC bridge P5083 and a three-electrode cell.

It is noticed that ionic conductivity of TBC membranes increases with PEO block lengthening from $6{,}2 \cdot 10^{-11}$ to $3{,}2 \cdot 10^{-9}$ $S \cdot cm^{-1}$. The introduction of additional ionic groups -COOH in polyethylene oxide/poly(acrylamide-*co*-acrylic) acid chains has a positive effect on the conductive characteristics of copolymer membranes. The ionic conductivity of TBC membranes filled with $LiPF_6$ increases with increasing of salt content.

The obtained results made it possible to consider PEO/PAAm triblock copolymers with interacting blocks as perspective matrices for producing solid electrolyte membranes and their possible application in Li-batteries, solar and fuel cells.

FEATURES OF THE OPERATION OF BIOSENSORS BASED ON THE PPR EFFECT IN CHROMATIC MODE

Kukla O.L., Fedchenko A.N., Vahula O.A., Surovtseva E.R., Shirshov Yu.M.
V.E. Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine
41, Nauki prosp., Kyiv, 03028, Ukraine, e-mail: kukla@isp.kiev.ua

Plasmon-polariton resonance (PPR) is a convenient physical effect for recording interactions of biological molecules on the surface of a thin metal film. Since the beginning of the 90s, many devices have been described for observing the specific and non-specific interaction of biomolecules with receptors fixed on the metal surface. And until now, this direction remains relevant, because thanks to the progress of genetic engineering there is a need for the creation of multichannel analyzers capable of simultaneously recording dozens of oligonucleotides in the analyzed mixture.

In this regard, it seems appropriate to develop a multichannel PPR device based on a chromatic analysis of the pattern of reflected light from a metal surface with a receptor template deposited on it. The reason for this is the expanded technical capabilities of using laser white light sources and small-sized webcams to register the color picture.

Currently, thin gold films are mainly used for sensory PPR applications; for this, surface chemistry methods have been developed for the controlled binding of ligands to the surface. However, the PPR effect in gold films is realized only in the red and IR spectral regions. At the same time, for an informative analysis of sensory interactions, it is desirable to use a wider range of wavelengths with registration of the main components of white light represented by the spectral components R, G, B. For this, it is necessary to analyze the suitability of other metals for the implementation of a chromatic PPR sensor.

In this paper, we simulated and analyzed the optical characteristics of reflection for a number of highly conductive metals (gold, silver, copper, aluminum, as well as gold and silver bilayers) under conditions of surface plasmon resonance in the Kretchman geometry. Of the metals considered, only thin silver films have the ability to realize a complete PPR in a wide range of wavelengths from 450 to 700 nm, covering the entire visible region of the spectrum for registration of biosensor reactions.

A method for the chromatic registration of adsorption by monitoring the R, G, B components of reflected light under conditions of PPR excitation from a white laser beam in a silver film 40-45 nm thick is proposed. The reflected light is directed to the RGB webcam recorder, which captures the image in X, Y coordinates. A pattern of ligands that specifically react with analyte molecules is preliminarily applied to the silver surface. In the experiment, the RGB (X, Y) distribution map is recorded before and after the interaction of the analyte and the ligand (receptor), and then a color difference analysis of these maps is performed.

EFFECT OF POST-PROCESSING ON THE EFFICIENCY OF PEDOT/PSS-Si SOLAR CELLS

Mamykin S.V., Lunko T.S., Mamontova I.B., Kondratenko O.S., Kotova N.V.
V.E. Lashkaryov Institute of Semiconductor Physics National Academy of Sciences of Ukraine
41, prospect Nauky, Kyiv 03680, Ukraine,
E-mail: mamykin@isp.kiev.ua

The PEDOT:PSS composite is a leading p-type organic polymer widely used to create photosensitive heterostructures of organic/inorganic semiconductor type. Such heterostructures are easy to manufacture thanks to low-temperature and vacuum-free technology and promising characteristics. The PEDOT:PSS in photovoltaic structures plays several roles. These are conductive front electrode, anti-reflective and passivating coating, charge-selective layer that reflects electrons and extracts holes, thereby significantly reducing recombination [1]. Currently, PEDOT:PSS/Si hybrid silicon-organic solar cells (SC) have been obtained with high solar energy conversion efficiency: 14.8% [2], 15.5% [3], 14.3% [4].

In SC of this type the intermediate SiO_2 plays a crucial role in the device performance because it increases the open circuit potential on the one hand. On the other hand, it has low conductance connected with tunneling, and if it is too thick, it blocks the current flow. Its growth over time is the main cause of the SC degradation. Thus, it should have the optimal thickness, but it is quite difficult to obtain it during device fabrication. In this work, we optimize the SiO_2 thickness by post-processing. Because the formed PEDOT:PSS film is porous, especially after washing out its PSS components, the PEDOT/Si separation boundary is readily accessible for chemical treatment. Post-processing of the fabricated PEDOT/Si structures was performed by treatment of the front surface of completely finished SC ether in an aqua solution of HF (10%) or a mixture of HF (10%) and $AgNO_3$ (0.8 mM) followed by few cycles of annealing and measuring of light current-voltage characteristics. Annealing was performed under ambient condition at 150°C for 15 s. During this process, the thickness of SiO_2 gradually increases. Efficiency increases to a certain limit and then begins to decline. The optimum was reached for etching of the front contact in 10% HF for 30 sec, followed by annealing at T=150°C for 30 sec. This formed a tunnel-thin intermediate layer of SiO_2, resulting in the efficiency of flat structures increased from 4.5% to 7.3% mainly due to the increase in the fill factor f and short-circuit current I_{sc}. Addition of $AgNO_3$ leads to the Ag nanoparticles deposition into the pores of the PEDOT layer. This reduces the serial resistance and increases the fill factor f further improving the photoconversion efficiency by 20%.

[1] P. Gao, Z. Yang, J. He, J. Yu, P. Liu, J. Zhu, Z. Ge, J. Ye, *Advanced Science.*, **2018**, 5, 1700547.
[2] S. Jäckle, M. Liebhaber, C. Gersmann, M. Mews, K. Jäger, S. Christiansen, K. Lips, *Scientific reports.*, **2017**, 7, 2170.
[3] Q. Liu, R. Ishikawa, S. Funada, T. Ohki, K. Ueno, H. Shirai, *Advanced Energy Materials.*, **2015**, 5, 1500744.
[4] J. He, P. Gao, Z. Ling, L. Ding, Z. Yang, J. Ye, Y. Cui, *ACS nano.*, **2016**, 10, 11525-11531.

POLY COMPLEXES BASED UNSATURATED β-DICARBONYLS AND LANTHANIDES FOR ORGANIC LIGHT-EMITTING DIODES

Savchenko I.O.[1], Berezhnytska O.S.[2,3] Ivakha N.B.[2,3], Trunova E.K.[2]
[1] *National Taras Shevchenko University of Kyiv,*
[2]*V.I.Vernadsky Institute of General and Inorganic Chemistry NASU*
Kyiv, Ukraine
[3]*National Technical University of Ukraine “Igor Sikorsky Kyiv Polytechnic Institute”, 37, Prosp. Peremohy, Kyiv 03056, Ukraine*
E-mail: iras@univ.kiev.ua

Unique luminescence features of trivalent lanthanide (LnIII) ions — sharp characteristic emission in the visible and near-infrared spectral regions, exceptional color purity, long luminescence lifetimes, high quantum yield and large Stokes shifts—afford them as promising electroluminescent materials [1]. Investigation of luminescent properties of coordination compounds of lanthanides, in particular β-dicarbonyls, is considerable practical interest, supported by the possibility of their use as luminescent materials [2-4].

Metallopolymers on the basis of Ln (III) complexes with new ligand - 2-methyl-5-biphenyl-1-pentendione-3,5 (mphpd) were obtained by radical polymerization. The copolymers with methylmethacrylate and styrene in a ratio of 5:95 are obtained. The kinetics of radical polymerization of synthesized metal polymers has been studied. The complexes were characterized by infra-red, absorption, diffuse reflectance and fluorescence emission spectra.

The spectroscopic studies of the synthesized compounds showed that the configuration of the chelate unit is unchanged during the polymerization.

By the luminescent spectroscopy is shown that all studied compounds exhibit effective luminescence.

[1] N. Wang, J. Wang, D. Zhao, Soren K. Mellerup, T. Peng, H. Wang, S. Wang, Lanthanide Complexes with Photochromic Organoboron Ligand: Synthesis and Luminescence Study, Inorg. Chem. 57(16) (2018) 10040–10049

[2] Zhou J., Whittell G., Manners I. Metalloblock Copolymers: New Functional Nanomaterials, *Macromolecules*, **2014**, 47,11, 3529-3543.

[3] Dzhardimalieva G, Uflyand I (2016) Metal Chelate Monomers as Precursors of Polymeric Materials, *J. Inorg. Organomet. Polym.*, **2016**, 26, 1112-1173.

[4] Luo J., Zhang C., Li C., Hua H., Hua B. Multiplicate sensitization of novel near-infrared luminescent linear copolymers based on Er, Nd and Yb-complexes, *RSC Adv*., **2014**, 4, 57393.

SYNTHESIS AND STUDIES OF PROPERTIES OF ORGANIC SEMICONDUCTORS CONTAINING DONOR AND ACCEPTOR MOIETIES

Levani Skhirtladze[1], Juozas Vidas Grazulevicius[1], Azhar Bin Ariffin[1,2], Woon Kai Lin[3]
[1]*Kaunas University of Technology, K. Donelaičio 73, LT-44249, Kaunas, Lithuania*
[2]*Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia*
[3]*Department of Physics, University of Malaya, 50603 Kuala Lumpur, Malaysia*
e-mail: levani.skhirtladze@ktu.edu

Organic light emitting diodes (OLEDs) have been a research focus due to their applications in display devices and general lighting. The maximal theoretical external quantum efficiency of fluorescent OLED is regarded to be of 5%, when assuming the out-coupling efficiency of 20%. On the other hand, phosphorescent materials can utilize triplet excitons in electroluminescence processes to achieve 100% internal quantum efficiency (IQEmax) [1]. However, the utilization of metals like iridium and platinum, which are expensive and nonrenewable, inevitably increase the cost of phosphorescent OLEDs. The materials exhibiting thermally activated delayed fluorescence (TADF) are noble-metal free fluorescent materials able to transform triplet excitons into singlet excitons through reverse intersystem crossing (RISC) to achieve 100% IQEmax in theory [2]. For TADF materials, the energy difference (ΔEST) between the first singlet excited state (S1) and the first triplet excited state (T1) must be small enough to enable the RISC process with the activation of environmental thermal energy [3]. To achieve this, electron donors (D) and electron acceptors (A) are introduced into the molecule to form an intramolecular charge transfer state with a large twisting angle between the donor and the acceptor to achieve the separation of highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO). Therefore, D–A-type or D–A–D-type molecules are the most classical TADF molecular structures.

In this work, new structures of organic emitters based 2,5-difluorobenzene acceptor moiety and the different donor units were designed. The structures of newly designed derivatives of 2,5-difluorobenzene and different donor fragments were estimated by DFT calculations using Gaussian software. HOMO-LUMO distributions were estimated, theoretical UV spectra were obtained and the energy differences of excited singlet and triplet states were calculated.

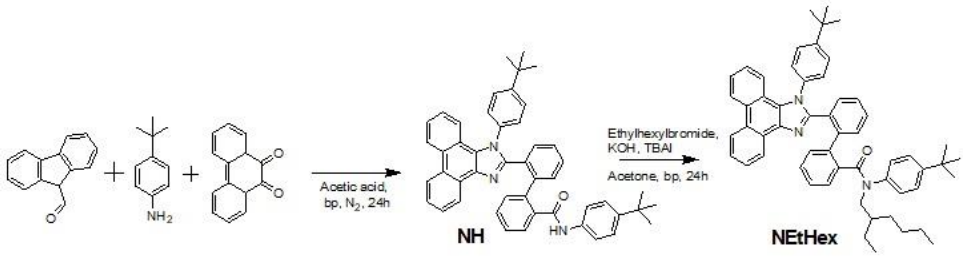
Acknowledgment. This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 823720.

References

1. Baldo, M. A.; Brien, D. F.; You, Y.; Shoustikov, A.; Sibley, S.; Thompson, M. E.; Forrest, S. R. *Nature* **1998,** *395,* 151–154. doi:10.1038/25954
2. Uoyama, H.; Goushi, K.; Shizu, K.; Nomura, H.; Adachi, C. *Nature* **2012,** *492,* 234–238. doi:10.1038/nature11687
3. Cai, X.; Li, X.; Xie, G.; He, Z.; Gao, K.; Liu, K.; Chen, D.; Cao, Y.; Su, S.-J. *Chem. Sci.* **2016,** *7,* 4264–4275. doi:10.1039/C6SC00542J

SYNTHESIS AND PROPERTIES OF PHENANTHROIMIDAZOLYL-BASED DERIVATIVES

Eigirdas Skuodis, Rokas Zubrevicius, Dmytro Volyniuk, Dalius Gudeika, Juozas V. Grazulevicius
[a] *Kaunas University of Technology, Department of Polymers chemistry and Technology,*
Barsausko 59, 51423 Kaunas, Lithuania
e-mail: eigirdas.skuodis@ktu.lt



Scheme 1

Derivatives of phenanthroimidazole are known as blue luminescent materials with high photoluminescence quantum yields, high charge drift mobilities, good morphological stabilities of their amourphous layers and as potential hosts and emitters for OLEDs [1, 2].

N-(4-t-buthylphenyl)-2’-(1-(4-t-buthylphenyl)-1H-phenanthro[9,10-d]imidazol-2-yl-N-(2-ethylhexyl)-biphenyl-2-carboxyimide (**NEtHex**) (**Sheme 1**) was synthesised in two steps. The structure of derivative **NH** was confirmed by X-ray diffraction analysis and all structures were confirmed by NMR and MS spectrometries. Compound **NEtHex** forms stabile molecular glass and exhibits high thermal stability. The photophysical and electrochemical properties of the synthesized compounds were explored. The theoretical values of HOMO, LUMO, singlet and triplet states energies of derivatives **NH** and **NEtHex** were calculated by Gausian software and compared with the corresponding experimental results.

Acknowledgement:
This project has received funding from the Research Council of Lithuania grant agreement No [P-LU-20-74].

References:

[1.]R. Butkute et al. *Dyes & Pigments* **2017**, 146, 425-437.
[2.]Zh. Wang et al. *J.Mater.Chem.*, **2011**, 21, 5451–5456.

IN SITU IMMOBILIZATION ON THE SILICA GEL SURFACE AND ADSORPTION CAPACITY OF POLY [8-METHACROYLOXYQUINOLINE] ON TOXIC METALS IONS

I. Savchenko[1], E. Yanovska[1], L. Vretik[1], D. Sternik[2], O. Kychkyruk[3]
[1]Taras National Taras Shevchenko University of Kyiv,60, Volodymyrska str., 01601 Kyiv, Ukraine
[2]Maria Curie-Skłodowska University, Maria Curie-Sklodowska Sq., 20-031 Lublin, Poland
[3]Ivan Franko Zhytomyr State University, 42 Pushkina Str., 10008 Zhytomyr, Ukraine
e-mail: iras@univ.kiev.ua

8-oxyquinoline is one of the most famous chelating agents, the first metal complexes of which have been known since the 19th century. 8-oxyquinoline is a group reagent because it interacts with approximately 40 metals to form soluble hydroxides or soluble hydroxo and amino complexes. The modification of the surface of porous inorganic materials by oxyquinoline-containing polymers allows to obtain sorbents for removing toxic metals from the waste water due to their complexation with nitrogen atoms of immobilized polymer. One of the promising ways of creating organo-mineral composite materials with valuable sorption properties is polymerization or *in situ* immobilization, which consists in the direct formation of an immobilized polymeric layer in the presence of particles of inorganic matrix. The advantages of this method of fixing a polymer on a solid surface in comparison with physical adsorption of pre-synthesized polymers are optimal location of macromolecules on a solid surface, which strengthens the fixation of a polymer on an inorganic matrix. This arrangement of macromolecules creates additional possibilities for the regeneration of the obtained composite material as a sorbent in multiple applications, and the possibility of self-organization of polymer chains in supramolecular structures on the surface of an inorganic matrix, the presence of which increases the sorption capacity of the composite. Compared to the chemical bonding of pre-synthesized polymers *in situ* immobilization is characterized by the absence on the solid surface of the matrix the residues of monomolecular compounds, which were used as bridging groups between the inorganic matrix and the polymer. All this leads to expansion of the range of immobilized polymer adsorption ability and improve its adsorption capacity.

This work is devoted to the *in situ* immobilization of poly [8-methacroyloxyquinoline] on the silica gel surface, and adsorption properties of the synthesized composite material on ions Pb(II), Cd(II), Zn(II), Mn(II), Cu(II) та Fe(III). The fact of polymer immobilization is confirmed by IR spectroscopy. The amount of immobilized polymer in the composition of the synthesized material is established according to thermogravimetric analysis. Using scanning electron microscopy, the surface morphology of the modified silica gel was established.

It has been found that the synthesized composite quantitatively removes from aqueous solutions the micro quantities of Cu (II), Mn (II) and Pb (II), and also exhibits high sorption activity against Zn (II) ions.

THERMALLY-STIMULATED LUMINESCENCE IN AN OLED HOST MATERIAL DOPED WITH TADF EMITTERS

Andrei Stankevich, Alexander Vakhnin, Andrey Kadashchuk
Institute of Physics, Natl. Academy of Sciences of Ukraine, Prospect Nauky 46, 03028 Kyiv, Ukraine
e-mail: andrei.stankevich@iop.kiev.ua

Thermally activated delayed fluorescence (TADF) is leading the third-generation technology of OLEDs. Due to promising characteristics, almost 100% internal quantum efficiency and the avoidance of rare and precious metals, TADF materials attract great research interest due to their potential application in displays and solid-state lighting. The energy disorder in a host-guest TADF layer affects its charge-transport properties and exciton formation pathways, which consequently influence the overall efficiency of an OLED device. Recent studies of TADF-based host-guest systems have revealed significant dependence of the energetic disorder in such layers on permanent dipole moments of host molecules and also on polarizability of guest molecules. In this work, we report on systematic study of charge trapping phenomena in TADF-based host-guest composition; namely, 3′,5-di(9H-carbazol-9-yl)-[1,1′-biphenyl]-3 (mCBP-CN) as a host matrix and 10-(4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl)-9,9-dimethyl-9,10-dihydroacridine (DMAC-TRZ) as a guest, using trap detection technique based on low-temperature thermally stimulated luminescence (TSL).

Principal results of this study are the following:

- Charge trapping in neat films is originated from the intrinsic localized states located within the tail of the Density-of-States distribution, which act as traps at sufficiently low temperatures.
- We obtained direct experimental evidence that DMAC-TRZ dopant creates a moderately deep extrinsic trap for electrons in mCBP-CN matrix.
- The key finding is that the average depth of the charge traps detected in the DMAC-TRZ-doped mCBP-CN films is not the exact difference between LUMO levels of host and guest materials, but depends significantly on dopant concentration. This implies that the charge trapping in such system is actually a cumulative effect of the intrinsic energetic disorder of the host and the extrinsic traps created by guest molecules.
- We demonstrated that the effect of DMAC-TRZ traps on TSL can be successfully described by the concept of ‘effective’ energy disorder σ_{eff} which is a function of intrinsic energy disorder σ_0 of the host, the trap depth, and trap concentration. Parameter σ_{eff} was experimentally evaluated for a set of mCBP-CN films doped with different DMAC-TRZ concentration. Surprisingly, σ_{eff} was found to feature a non-monotonous behavior - it first increases with increasing trap concentration, and then decreases when trap concentration exceeds ~1wt%. This quantitatively agrees with predictions of hopping transport model developed before for trap-containing materials.

The authors acknowledge funding through the EU Marie Skłodowska-Curie ITN ‘TADF*life*’ grant (GA no. 812872).

ON THE NATURE OF CURRENT CARRIERS IN INTERPOLYMER COMPLEXES PEDOT:PSS AS COMPONENTS OF SOLAR CELLS

O.I. Tkachuk, M.I. Terebinska, Ya.S. Krivoruchko, V.V. Lobanov
Chuiko Institute of Surface Chemistry of National Academy of Sciences of Ukraine,
17 General Naumov Str., Kyiv, 03164, Ukraine,
E-mail: tkachuk_olya@bigmir.net

In the recent past, the interpolymer complex of poly(3,4-ethylenedioxythiophene) with polystyrene sulfonic acid (PEDOT:PSS) is studied extensively. Unique properties of the latter such as good film forming ability, excellent optical transparency in the visible range, high electroconductivity in its oxidized form, and power conversion efficiency have stimulated an interest to the theoretical investigation of its electronic properties.

In this study we present the results of quantum-chemical calculations (DFT, B3LYP, 6-31 G**) of (i) 3,4-ethylenedioxyethylene (EDOT) oligomers containing 2 to 12 units in the oxidation states 0, +2, and +4; (ii) styrene sulfonic acid (SS) oligomers consisting of 2 and 4 units in their charged states 0, -2 и -4; (iii) electroneutral EDOT:SS complexes.

We have shown that the energy difference between HOMO and LUMO (ΔE) amounts 2.25 eV for the $(\mathrm{EDOT})_8$ oligomer, while decreasing to 1.09 eV for the $(\mathrm{EDOT})_8^{2+}:(\mathrm{SS})_2^{-2}$ complex, and further to 0.73 eV for the larger $(\mathrm{EDOT})_8^{4+}:(\mathrm{SS})_4^{-4}$ complex. Such a reduction of ΔE evidences in favour of the increased electric polarizability and electroconductivity of doped oligomer complexes as the doping degree increases.

Our calculations have also shown for the oxidized EDOT chains consisting of more than 12 units to be more stable when two polarons are situated at their ends, as compared to the configuration with one four-membered polaron at the centre of the chain.

We have also concluded that the bipolaron creation is energetically more favourable than the formation of polaron pairs for short oligothiophene cations, while both the bipolaron and the polaron pair contribute significantly to the structure of the current carrier in medium-sized oligothiophenes (up to 10-12 units). For longer oligomer cations, the polaron pair dominates. Experimental data available in literature do not allow one to make an unambiguous conclusion in favour of either bipolarons or monopolaron pairs.

COMBINED POLYMER SENSITIVE ELEMENTS FOR GAS SENSORS

O. Aksimentyeva[a], B. Tsizh[b,c], Yu. Horbenko[a], M. Dzeryn[c]
[a] *Ivan Franko Lviv National University, 6 Kyryla-Mefodia, 79005, Lviv, Ukraine*
[b] *Kazimierz Wielki University in Bydgoszcz, 30 Chodkiewicza, Bydgoszcz, 85-064, Poland*
[c] *Stepan Gzytsky Natoinal University of Veterinary Medicine and Biotechnologies Lviv, 50 Pekarska, 79010, Lviv, Ukraine*
e-mail: tsizhb@ukw.edu.pl

Today, intensive search for materials and structures of the sensitive elements of gas sensors is being carried out to improve their performance. In recent years, there has been an increasing interest in the usage of gas-sensitive polymer films in gas sensors due to their better processability, ease of synthesis and use, lower cost, and in some cases, better performance. Many authors have shown that the optimal sensing elements of this class are thin films of electrically conductive polyaminoarenes, in particular, polyaniline and its derivatives, including composite nanostructures based on them [1-5].

Improving the values of sensitivity, selectivity, reversibility, reproducibility and other parameters of gas sensors using sensitive polymer films can be achieved through a number of modification methods, in particular, the creation of thin-film combinations of different chemical composition of electrically conductive polyaminoarenes. This superposition extends the functionality of the active elements and improves the performance of the gas sensors based on them. Previously, we have already shown that the thin film bilayer structures of polyaniline/poly-3,4-ethylenedioxythiophene significantly expand the spectral sensitivity range of the respective sensing elements compared to the monolayer films [4].

At this stage, we have developed a gas-sensitive combination polymeric active element for gas sensors based on a mixture of polyorthoanisidine (PoA) and polyortotoluidine (PoT). We have investigated the optical absorption spectra of thin films electrodeposited from a solution of monomer mixtures (PoT + PoA, 1:1). It is shown that the absorption of the obtained films varies more significantly than one of the individual components due to the action of ammonia, carbon dioxide, vapor of hydrogen sulfide and other volatile substances in the wide spectral range from 350 to 900 nm, which provides the application of synthesized combined structures for the manufacture of optical sensors.

1 S. Pandey. *J. Sci.: Advanc. Mater. Devices,* **2016**, 1, 431.
2 S.J. Park, C.S. Park and H. Yoon. *Polymers,* **2017**, 9, 155.
3 B.R. Tsizh, O.I. Aksimentyeva, Ya.I. Vertsimakha et al. *Mol. Cryst. Liq. Cryst.,* **2014**, 529, 116.
4 B.R. Tsizh, O.I. Aksimentyeva, *Mol. Cryst. Liq. Cryst.,* **2016**, 639, 33.
5 O.I. Aksimentyeva, B.R. Tsizh, Yu.Yu. Horbenko et al. *Mol. Cryst. Liq. Cryst.,* **2018**, 670, 3.

EXCIPLEX-BASED APPROACHES FOR WHITE LIGHT EMITTING DIODES

Dmytro Volyniuk, Galyna Sych, Matas Guzauskas, Jurate Simokaitiene, Juozas V. Grazulevicius
Department of Polymer Chemistry and Technology, Kaunas University of Technology,
Barsausko 39, LT- 51423, Kaunas, Lithuania;
e-mail: dvolynyuk@gmail.com

Commonly, charge and exciton recombination zones are distributed within the same light-emitting layers in white organic light-emitting layers (OLEDs) leading to device stability decrease because of the triplet–triplet and/or exciton-polaron annihilation processes. There are approaches for white OLEDs described in the literature which propose to separate charge and exciton recombination zones [1, 2]. However, exciton energy transfer between two separated by spacer TADF emitters was not reported yet due to the best of our knowledge. Long-distance energy transfer, i.e. transfer of triplet excitons with long diffusion lengths, from one TADF emitter to another one is not expected since direct harvesting of triplet excitons through revers intersystem crossing (RISC) take place in TADF emitters. Nevertheless, we observed separation of charge and exciton recombination zones between two separated by spacer TADF emitters including exciplex-based one. Thus, capability of long-distance energy transfer of exciplex through a spacer (>20 nm) under electrical excitation was detected for the first time in this study.

Based on this observation, we propose an approach towards exciton distribution between exciplex-based cyan and orange TADF emitters for white electroluminescence of enhanced stability. We present three effectives thermally activated delayed fluorescence exciplex systems formed between newly synthesized cyanocarbazolyl derivatives as electron-donors with commercially available electron acceptor PO-T2T and demonstrate their application in OLEDs. The newly synthesized cyanocarbazolyl derivatives exhibited high energy of triplet levels ranging from 2.90 eV up to 3.04 eV and bipolar charge transport favourable for effective exciplex-formation. Proper alignment of long-lived triplets of the spacer and the exciplex systems allowed to implement exciplex energy transfer through the spacer and its recombination in the layer of TADF compound 2,3,5,6-tetrakis (3,6-diphenyl-9H-carbazol-9-yl)-1,4-benzenedicarbonitrile or the red iridium complex Ir(piq)$_2$(acac). We fabricated efficient single-color and white devices with new exciplex-forming systems and achieved maximum external quantum efficiency of 7.7 %. We obtained warm white electroluminescence with CIE coordinates of (0.36, 0.44) exploiting cyan intermolecular (exciplex) and orange intramolecular thermally activated delay fluorescence.

Acknowledgements. This work was supported by the Research Council of Lithuania within scientific co-operation program between Lithuania and Ukraine (“LUW”, S-LU-20-9).

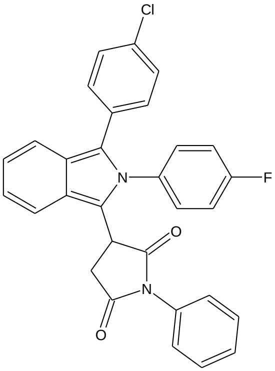
[1] S. Reineke, F. Lindner, G. Schwartz, N. Seidler, K. Walzer, B. Lüssem, K. Leo. *Nature*, **2009**, 459 (7244), 234.

[2] F. Zhao, Y. Wei, H. Xu, D. Chen, T. Ahamad, S. Alshehri, Q. Pei, D. Ma. *Mater. Horiz.*, **2017**, 4, 641–648.

3-[3-(4-CHLOROPHENYL)-2-(4-FLUOROPHENYL)-2*H*-ISOINDOL-1-YL]-1-PHENYLPYRROLIDINE-2,5-DIONE AS A CANDIDATE FOR SOLAR CELLS APPLICATIONS

A. El Haimeur[a,b], I. V. Levkov[b], T. V. Yegorova[b], A. I. Kysil[b], H. Bakkali[a], E. Blanco[a],
Z. V. Voitenko[b]
[a] *Department of Condensed Matter Physics and IMEYMAT: Institute of Research on Electron Microscopy and Materials, University of Cadiz, Campus Universitario de Puerto Real, E11510 Puerto Real, Cádiz, Spain*
[b] *Department of Organic Chemistry, Faculty of Chemistry, Taras Shevchenko National University of Kyiv, Volodymyrska Street, 64/13, Kyiv 01601, Ukraine*
e-mail : tve2008@ukr.net

Recently, several new materials based hydrocarbon systems are friendly with the environment were used in organic solar cells and have been studied and developed [1] due to their easy preparation and low cost price to combine between the criteria cost/perfomance which decrease the price of the technological devices. In the past few years, the importance of the organic π-conjugated molecules rises due to its large domain applications in the fields of chemistry and materials engineering.



We report new synthesized materials: the isoindole derivative with donor-acceptor structure. The material has been characterized by X Ray Diffraction, SEM and UV-Vis absorption. The band structure of the molecular system was investigated by DFT calculations and reported for the first time. The computed results of the organic compounds revealed the isoindole derivative can be applied as an electron transporting layer in organic bulk heterojunction (BHJ) and it can be applied in nonlinear optical device.

[1] J. Zhao, Y. Li, G. Yang, K. Jilang, H. Lin, H. Ade, W. Ma, H. Yan, *Nature Energy*, **2016**, 1, 15027.

NEW MATERIALS BASED ON COMPLEXES AND METALOPOLYMERS OF EUROPIUM (III)

Berezhnytska O.S.[a,b], Rohovtsov O.O.[a], Fedorov Ya. V.[a], Savchenko I.O.[c], Trunova O.K.[a]
[a] *V.I.Vernadsky Institute of General and Inorganic Chemistry of NAS of Ukraine, Akad. Palladin Avenue, 32/34, Kyiv, Ukraine, 03142*
[b] *National Technical University of Ukraine «Igor Sikorsky Kyiv Polytechnic Institute», 37, Prosp. Peremohy, Kyiv, Ukraine, 03056*
[c] *National Taras Shevchenko University of Kyiv, 64/13, Volodymyrska Street, Kyiv, Ukraine, 01601*
e-mail: olekberez@gmail.com

Metal-polymer and hybrid materials have attracted the attention of researchers, which is due to the wide range of their properties, and, accordingly, the areas of application. They can be used as solutions and powders, as well as films of different thicknesses. An important aspect of the study, both from a fundamental and applied point of view, is to study the influence of the nature of the ligands on the spectral-luminescent properties of the compounds. Therefore, the synthesis and study of the physicochemical properties of lanthanide coordination compounds based on β-diketones with multiple bonds, which makes it possible to obtain new polymeric materials based on them, is an up-to-date study of modern chemical science.

Most studies are based on the preparation of metal-polymers by intercalating metal salts into polymer matrices. This method does not allow to obtain a homogeneous chemical composition of the compound, which causes both heterogeneity of the materials and their aggregation in the production of films. We are offering another approach to solve this problem.

As ligands, the use of β-diketone compounds containing unsaturated substituents in chelate rings are proposed. The presence of a double bond in the molecule allows the use of these compounds as monomers in the polymerization reaction. In this way, the coordination compounds of lanthanides can act as precursors in the reactions of radical homo- and copolymerization. The production of copolymers of lanthanide complexes with industrial monomers (methyl methacrylate, styrene, vinyl carbazole, unsaturated carboxylic acids) will improve the physico-chemical characteristics (thermal stability, flexibility) and reduce the cost of final products. The variation of the composition of the copolymer allows to expand the spectrum of their practical application, to increase the functionality of the material.

Europium (III) complexes were obtained on the basis of the three ligands. Radical homopolymerization produced metal polymers. In order to determine the composition and structure, all the synthesized compounds were investigated by physico-chemical methods of analysis. It is shown that the coordination number of Eu(III) ions in the synthesized compounds is 8. It is established that polymerization does not cause a significant change in the coordination polyhedron. Studies of luminescent properties have shown that the luminescence intensities of complexes based on mbphpd and mphpd are the highest, due to both the more hard structure of these molecules and the additional antenna effect created by phenyl substituents. The maximum luminescence efficiency is characteristic of the metal polymers Eu (III) and Tb (III).

PROPERTIES OF POLYHEXAFLUORPROPYLENE THIN FILMS

K. Grytsenko[a*], Yu. Kolomzarov[a], P. Lytvyn[a], V. Ksianzou[b], S. Schrader[b]

[a]V.E. Lashkaryov Institute of Semiconductor Physics, pr. Nauki 41, Kyiv, Ukraine
[b]Institute of Photonics, Laser & Plasma Technology, University of Applied Sciences Wildau,
Hochschulring 1, Germany
e-mail: d.grytsenko@gmail.com

Perfluoropolymer thin films are used mainly as protective coatings, but recently started to use as barrier layer in organic light emitting diodes and organic transistors [1]. Polyhexafluoropropylene (PHFP) was heated to decomposition temperature in vacuum. The emitted fragments of polymer chain went through a cloud of accelerated electrons and condensed on a substrate. Electron cloud enhanced film deposition rate by five times. Mass-spectra showed that upon activation concentration of all ions was not significantly changed. Infrared spectroscopy (IRS), atomic force microscopy (AFM) and spectral ellipsometry showed, that structure of the PHFP deposits is close to the structure of the bulk PHFP. Surface relief and refractive index of the PHFP film are shown in Figure. The film is transparent, uniform and continuous with surface roughness at nanoscale. The surface of the film seems as composed from “islands” up to 500 nm in size, which, in turn, are composed from smaller units about 30-100 nm in size. The refractive index is almost the same for the films of 55 nm and 173 nm thickness, indicating isotropic structure of the films.

Thin PHFP films can be used in OLEDs, optical and electrical sensors, etc integrated optical devices as transparent, barrier, dielectric and protective layers.

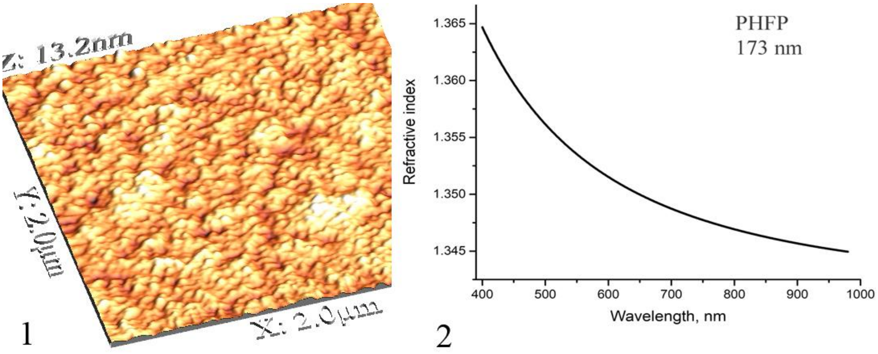


Figure. 1 - surface relief, 2 - refractive index of the PHFP film.

[1] V. Yaschchuk, K. Gytsenko, S. Schrader, O. Navozenko, *Bulletin of Kyiv Univ., Ser.: Phys. Mathematics*, **2017**, 109-118.

BIOLOGICALLY ACTIVE COMPOUNDS BASED ON SILVER COMPLEXANTS

Myhalchuk A.O.[a], Sikors'ka K.A[a], Kamenska T.A.[a], Berezhnytska O.S.[a,b]

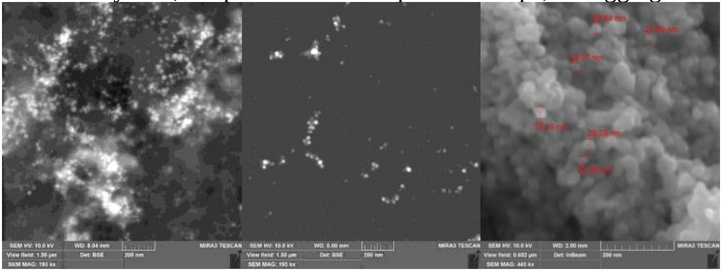
[a] *National Technical University of Ukraine «Igor Sikorsky Kyiv Polytechnic Institute», 37, Prosp. Peremohy, Kyiv, Ukraine, 03056*

[b] *V.I.Vernadsky Institute of General and Inorganic Chemistry of NAS of Ukraine, Akad. Palladin Avenue, 32/34, Kyiv, Ukraine, 03142*

e-mail: olekberez@gmail.com

Over the last decades, the development of nanotechnology has reached its height. Of particular interest to researchers are nanoparticles of metals, which have different properties (conductive, optical, magnetic). It is known that the properties of nanosystems are directly related to the size of the dispersed phase nanoparticles. Therefore, studies in the field allow direct synthesis, by obtaining particles of a certain size with the desired properties. The relevance of research based on the targeted synthesis of substances, systems or particles of a given composition, size or shape with specified properties is steadily increasing. With the development of science, requirements for synthetic chemistry and the need for practical application of synthesized compounds are changing. Today it is no longer relevant to obtain new compounds or systems unless they have "special" properties and applications. Silver nanoparticles, or as they are called colloidal silver, is an interesting and unique antibacterial agent that has been proven by many researchers. They are used in biotechnology, bioengineering, cosmetology, pharmaceuticals and even food.

Basically, to obtain silver nanoparticles, known methods of silver recovery are used which consist in the recovery of salts in a certain environment with the use of surfactants. These include citrate, boron hydride, glucose, aniline and other methods. This method consists in recovering the metal salt in a particular medium in the presence of surfactants using different reducing agents. Relevant in our opinion is the synthesis of silver complexate and obtaining on its basis a nanodispersed system stabilized with a solution of trilon-B in order to obtain an antibacterial additive. Ethylenediaminetetraacetate of silver (I) was obtained. It is shown that the concentration of $5\cdot 10^{-2}$ M, pH = 5-6, 2: 1 reagents is the optimal conditions for obtaining the silver complexant. The set of physicochemical methods of analysis (SEM, ESP, dynamic light scattering) shows that the obtained systems are nanodispersed, and the particle size is in the range of 22-30 nm, there is practically no agglomeration in the system, the particles have a spherical shape, are aggregate stable.



SEM microphotography of solution and powder $Na_3[Agedta]$

SELF-ASSEMBLED DICHROIC ORGANIC SOLIDS

K. Grytsenko[a], P. Lytvyn[a], Y. Kolomzarov[a], Y. Slominskii[b], V. Kurdiukov, O. Navozenko[c]

[a]V. Lashkaryov *Institute of Semiconductor Physics, pr. Nauky 41, Kyiv, 03650, Ukraine*
[b]*Institute of Organic Chemistry, Murmanska str. 5, Kyiv, 02660, Ukraine*
[c]*T. Shevchenko National University 64/13 Volodymyrska Str., 01601, Kyiv, Ukraine*
[a] d.grytsenko@gmail.com

Oriented organic films were produced long ago by different aligning methods. The aligning sublayer was used for production of oriented films of metals, polymers, liquid crystals and small molecules (dyes). Recently the polytetrafluorethyle (PTFE) sublayers, deposited in vacuum and rubbed with a cloth (RVD) were used for oriented growth of organic dye films. Several modifications of squaraine dyes produced oriented dichroic films on RVD PTFE by self-assembly by deposition in vacuum [1,2]. The properties of the dichroic films are dependent on the molecule used and characteristics of the sublayer. We found out, that several dyes formed nanowires without aligning sublayer just by self-assembly [3]. A few of these dyes formed dichroic nanowires. If micro-stripped unidirectionally ordered substrate was used, the dye dichroic nanowires were grown in oriented manner both on gold strips and between them. The paper presents data concerned influence of dye and sublayer structure on the morphology and optical propertied of the dichroic deposits.

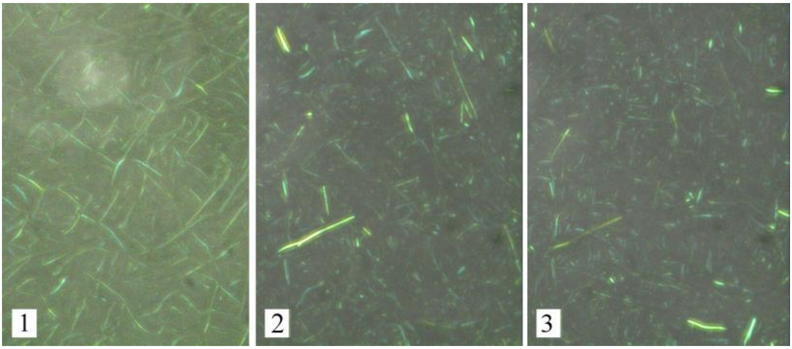


Figure. Dye nanowires: 1 – on glass, 2 - and 3- on gold with crossed polarizers.

[1] K. Gritsenko, D. Grinko, O. Dimitriev, S. Schrader, A. Thierry, J.C. Wittmann. *Optical Memory and Neural Networks,* **2004,** *3*, 135-143.
[2] K. Grytsenko, O. Lytvyn, V. Bogutskii, R. Velagapudi, V. Ksianzou, S. Schrader. In *Abstr. Book: Winter School on Organic Electronics*, Planneäralm, Austria, **2007**, 62.
[3] K. Grytsenko, P. Lytvyn, Y. Slominskii, *J. Appl. Phys. A*, 125, **2019**, 406 - 422.

SYNERGETIC EFFECT STUDY IN TWO-COMPONENT MIXTURES OF ASCORBIC ACID WITH AMINO ACIDS

Hocharenko A.[a], Chygyrynents O.[a]
[a] *National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute"*
37, Peremogy Ave, 03056, Kyiv, Ukraine
e-mail: nastiagoncharenko55@gmail.com

Amino acids are used as antioxidants. The most famous are histidine, arginine, asparagine and others. In humans, histidine is an important chemical compound that promotes protein metabolism and is involved in the formation of red and white blood cells contained in hemoglobin.

Two antioxidants, which differ significantly from the energy of dissociation of the bond, are related to synergistic antioxidants [1]. At least 0.01 ~ 0.02% of ascorbic acid is required to obtain a significant synergistic effect with δ-tocopherol in the stabilization of fish oil. Such amino acids are capable of interacting with the formation of complexes with certain reagents, such as phosphomolybdenum, by methods such as the reduction of iron, the oxidation of crocin [2].

Ascorbic acid is the most active antioxidant, at the same time, amino acids in the individual state exhibit insufficient activity. Therefore, purpose of work is to study the synergistic effect of mixtures of amino acids with ascorbic acid and to study the effect of amino acid structure on antioxidant activity.

From the data obtained, it is shown that the optical density of mixtures of amino acids with ascorbic acid is intensively increasing in comparison with the individual compounds. The maximum optical density A_{max} in the mixture of ascorbic acid and L-histidine is observed at the ratio Asc: L-His = 2:3 ─ 1,191, in the mixture of ascorbic acid and L-carnitine ─ 1,193 at Asc: L-Kar = 3:7, in a mixture of ascorbic acid and methionine ─ 1,148 at Asc: Met = 3:7, in a mixture of ascorbic acid and L-serine ─ 0,249 at Asc: L-Ser = 2:3, in a mixture of ascorbic acid and L-lysine ─ 0,602 at Asc: L-Lys = 3:2.

The synergistic efficiency of amino acids with respect to ascorbic acid is reduced in the range L-Kar> L-His> L-Met> L-Lys> L-Ser. The analysis of the obtained results shows that in the mixtures of the test substances there is a phenomenon of synergism.

References

1. M.Koushki, M. Nahidi Physico-chemical properties, fatty acid profile and nutrition in palm oil, *J.Paramed. Sci*, **2015**, v.6, p. 117-134.

2. F.Tubaro, A.Ghiselli, P.Rapuzzi, M M.aiorino, F. Ursini Analysis of plasma antioxidant capacity by competition kinetics, *Free Radicals in Biology and Medicine.*, **1998**, v. 24, p. 1228–1234.

LASER TEXTURING OF SILICON SOLAR CELLS AS AN ALTERNATIVE TO CHEMICAL WET ETCHING

O. Candemir[a], E. Genc[b], H. Ciftpinar[b], H. Nasser[b], M. Zolfaghari Borra[b], A. Bek[a, b], R. Turan[a, b], I. Pavlov[a, b]

a. Department of Physics, Middle East Technical University, 06800 Ankara, Turkey

b. Center for Solar Energy Research and Application, Middle East Technical University, 06800 Ankara, Turkey

e-mail: ozuncan@gmail.com

Si-based solar cell (SC) constitute the main source of the solar energy in the world. The conventional way to minimize thermodynamic losses for the high efficiency Si-based photovoltaic devices, is photonic design of the device surfaces, which is usually done by chemical anisotropic etching. Unfortunately, the last one increases the cost per watt for the final device, and arises additional environmental issues.

Recently, a new method, Nonlinear Laser Lithography (NLL) [2], was developed for laser-induced periodic surface structuring, which allows nanostructuring of indefinitely large areas of many materials by excellent periodicity and uniformity.

In present work we report the creation of photonic structure on Si-based SC by using NLL technique. As a laser source we used home-made femtosecond laser system, operating at 1030 nm. The laser beam was focused on Si surface (single crystalline p-doped wafer, with 1-3 Ω·cm resistivity and thickness – 300 μm) and raster scanned with galvo-scanner. SEM image of the structure is represented in fig 1(a).

The SC`s were produced on structured, unstructured, and conventionally textured wafers. The p-n junction was formed by phosphorous diffusion in doping furnace, followed by silicon nitride passivation coating, and back and front surface metallization in order to form electrical contacts. The maximum efficiency ~15% was obtained for the laser structured samples.

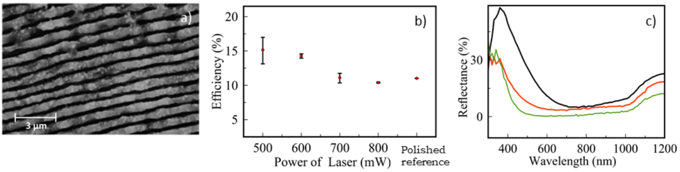


Fig. 1 (a) – SEM image of 1x1 cm^2 structured area; (b) – efficiency measurements for structured areas with different powers and unstructured sample (as a reference); (c) – reflectance measurements for structured areas with different powers (black - 500 mW, red - 600 mW, green - conventionally textured reference).

We expect this technique to be successfully applicable in the future in SC industry as an alternative for conventional chemical wet etching.

[1] A. Polman and H. A. Atwater, Nature Materials *11*, (2012), 174.
[2] B. Öktem, I. Pavlov, S. Ilday, H. Kalaycıoğlu, A. Rybak, S. Yavaş, M. Erdoğan and F. O. Ilday, Nature Photonics *7*, (2013), 897.

We acknowledge *Scientific and Technological Research Council of Turkey* (TÜBİTAK) Project No 118F375

PHOTOCONDUCTIVITY IN POLYETHYLENE-SEMICONDUCTOR (p-GaSe) COMPOSITE

Babayeva R.F.[1], Abdinov A.Sh.[2], Amirova S.I.[2]
[1]*Azerbaijan State University of Economics (UNEC),*
[2]*Baku State University*
e-mail: babaeva-rena@yandex.ru

Features of photoconductivity of composite materials such as polymer matrix-semiconductor filler is of interest from both practical and fundamental points of view. Because in terms of their transport and generation-recombination properties, photosensitive composites under certain external conditions, located in the middle between spatially homogeneous crystalline and single-phase non-crystalline substances, have wider possibilities for varying physical properties. In the present work, the goal was a comprehensive experimental study of photoconductivity in a composite consisting of a polymer matrix and a semiconductor filler: a high density composite polyethylene – layered semiconductor of gallium monoselenide (p-GaSe)

The choice of p-GaSe semiconductor as a filler was due to its high chemical resistance and photosensitivity in the entire visible region of the optical spectrum, and the choice of high density polyethylene as a matrix was due to a good study of the electrophysical properties of this polymer.

The photoconductivity kinetics when turned on by light has a fast relaxing (with a time constant of no more than $\sim 10^{-(5-6)}$ seconds), and when the light is turned off, it has a slow relaxing (depending on N, U_0. values and with a time constant varying within 1-6 seconds) character.

The relaxation of photoconductivity after the exposure to light is turned off, similarly to the case when the additional current is quenched in tunneling diodes, due to the recombination of nonequilibrium charge carriers by overcoming a certain recombination barrier at the interface between the polymer matrix and the semiconductor filler, therefore, the time constant gradually increases during this process.

According to all the revealed signs, the photoconductivity found in the composite under study has an induced character and is due to the emptying of the nonequilibrium-filled capture levels existing in the quasi-forbidden zone of the matrix when exposed to light. Non-equilibrium filling of these levels is carried out by their capture of nonequilibrium charge carriers injected at certain values of U_0 through current contacts and (or) created by light in a photosensitive semiconductor filler.

Based on high density polyethylene and p-GaSe semiconductor, it is possible to create a polymer-semiconductor composite photosensitive in the visible range of the optical spectrum.

PHOTOELECTRET EFFECT IN POLYMER-PHOTOSENSITIVE SEMICONDUCTOR n-InSe COMPOSITES

Dzhafarova S.Z.[1], Babaeva R.F.[1], Ragimova N.A.[2], Abdinov A.Sh.[2]
[1]Azerbaijan State University of Economics (UNEC),
[2]Baku State University
e-mail: exiton_1992@mail.ru

The paper reports on the results obtained in experimental studies of the photoelectrical properties of a composite consisting of high density polyethylene and a layered semiconductor of indium monoselenide (n-InSe). The studied samples were cut from thin (0.100≤d≤0.120 mm thick) composite films with different volume percentages (N=10-50 vol.%) of n-InSe.

In the samples under study, the dependences of the photoelectret potential (U_e) and its relaxation time (τ_{phe}) on the content of the semiconductor filler in the composite (N) were measured for various exposure durations (t_p) and electric field strengths (E_p), light intensity (Φ_p), and temperature (T_p).

After prolonged conservation under the influence of a constant electric field, intense illumination, at high temperatures at constant values, a photoelectret state is formed in the samples under study.

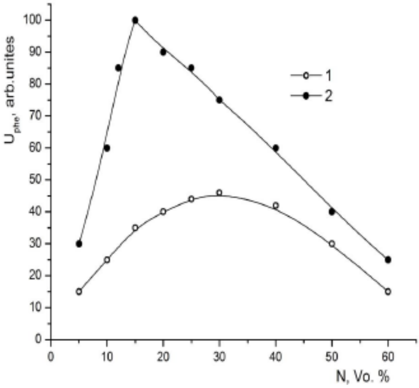


Figure 1. tp=2.4·10^3 c; Tp=300 K; Ep=3·10^{1}V·sm^{-1}; Φp=3.6·10^2 mVt·sm^{-2}

Pre-treatment of the polymer matrix in a gas discharge significantly improves the photoelectrical parameters and characteristics of the studied composite.

The value of the photoelectrical potential difference (Ue) non-monotonously depends on the content of the filler (N) and, at a certain value, reaches its maximum value.

The value of N, corresponding to the maximum of the dependence $Ue(N)$ and the relaxation time formed at different modes of the photoelectrical state, differ from each other, and do not depend on the direction of the constant electric field applied to the sample under study

AUTHOR INDEX

A

Abdinov A.Sh. 344. 345
Abdinova G.D. 94, 179
Abdullayeva I.A. 94
Afanasyev D.A. 176
Agayev T.N. 177
Aghazade A.I. 209
Akhmedova A.M. 177
Akhundova N.M. 179
Aksimentyeva E.I. . 144
Aksimentyeva O. 119, 121, 138, 316, 320, 335
Alakbarova T.M. 268
Alekberov R.I. 93
Alekseev O. 250
Alekseeva T.T. 178
Alieksandrov M.A. 103
Aliev Z.S. 268
Aliyeva T.D. 179
Andriiko O. O. 217
Andriyevsky B. 66
Androulidaki M. 52
Andrulevicienė V. 315
Anoshenko M. 65
Antonenko O. 232
Antonenko O.I. 105
Antonyuk N. 75
Antypov I. 300, 313
Apostolova R. 57
Ardjoum N. 196
Artemenko A. 174
Ariffin A. 315
Ariffin A.B. 330
Aslanov A. 154
Astakhova O. 81, 180
Astrelin I. 234
Atayeva S.U. 50, 159
Aurbach D. 57
Averchenko K. 277
Azhniuk Y.M. 51, 129

B

Babanly M.B. 181, 209, 219, 253, 268
Babčenko O. 174
Babenkov E.A. 77
Babkina N. 232
Babuka T.Ya. 227
Bagiyeva G.Z. 179
Bakkali H. 170, 337
Balevicius V. 40
Bandura Kh. 216
Baran J. 204, 205
Baran N. 184
Barbash V. 52, 71
Barbash V.A. 69
Barkhalov B.Sh. 179
Bakhtiyarly I.B. 219
Barylo H.I. 18
Baumer V.N. 228
Bayramova U.R. 181
Bazylyuk T. 65
Blashkiv O. 278
Bei I. 182
Bek A. 160, 162, 183, 189, 343
Belous A. G. 220
Berest V.P. 280
Berezhnytska O.S 329, 338, 340
Berezhnyy B. 184
Berezovska N. 197
Berezovska N.I. 157
Berezovskaya I.V. 104, 112, 261
Bernard R.S. 315
Bespalova I. 140, 154
Bevzo V. 14
Bezrodna T.V. 105, 141, 232
Bezrodnyi V.I. 105, 141, 232
Bezvikonnyi O. 175, 207, 256, 315, 317
Biliuk A.A. 106
Bilyk S. 313
Bilogubka O. 185
Blanco E. 170, 337
Bratychak M. 81, 180, 191, 310

Blazevicius D. 186, 323
Blazhynska M.M. 32
Bliznyuk V. 139, 240
Bliznyuk V.N. 173, 187
Blonskyi I. 197
Bogatyrov V.M. 148
Bogoslovska A. 188
Bondar O.O. 201
Bordyuh H. 165
Borets A. 70
Borkovska L. 107, 318
Borova M. 279
Bortchagovsky E.G. 53, 56, 108, 188
Borynskyi V.Yu. 64
Boryseiko O. 10
Borysenko M. 200
Bovgyra O. 55, 66
Boychuk V. 216
Boyko D.V. 20
Boyko I. 109
Boyko V. 250
Brazhnyk D.V. 80
Brizhik L. 9
Brodin O.M. 167
Brodyn M.S. 167
Brovarets V. 230
Brovarets V. S. 26, 131
Brovko O.O. 105
Bruzaud S. 276
Brychenko I. 202
Bucinskas A. 175, 321
Budianska L.V. 280
Budzinska V. 65, 182
Bugaychuk S. 165
Bukhinik O. 192
Bukivskii A.P. 110, 201
Bukivskii P.M. 110, 201
Bulavin L.A. 136
Bunyakina N. 198, 225
Burlachenko J. 319
Burlakov V.O. 54
Busko T. O. 22, 97, 100

C

Candemir O. 160, 343
Cardin J. 318
Cekaviciute M. 193, 206
Çınar K. 183
Ciobanu M. 58, 86
Chaban O. 42
Chabecki P. 156
Charnyi D.V. 97, 100
Chavhan S. 323
Chayka M. 307
Chibani N. 196
Chigvintseva O. 264
Chegel V.I. 22
Chekhun V. 292
Chepurna O.M. 269
Chernii S.V. 296
Chernii V.Y. 296
Chernykh S.I. 251
Chetrus P. 76
Chisca D. 4
Chmil A. 28
Chomicki D. 164
Chornenka N. 36, 296
Chornous V. O. 211
Chornyi V.S. 291
Chuenko R.M. 282
Chudoba D. 136
Chuprina N.G. 62, 87
Chygyrynents O. 342
Cociu V. 4
Coropceanu E. B. 239
Croitor L. 4

D

Dai F. 108
Danilenko I. 124
Davidenko I. 62, 87
Davidenko N. 62, 87, 218, 221
Datsko T. 194
Degoda V. 40, 293

Dehouche N. 276
Demchenko A.P. 95
Dementjev A. 13, 29, 205
Demianenko E.M. 111, 118
Demydenko Yu.V. 56
Denis L.V. 22
Derevyanko N.A. 187
Derkowska-Zielinska B. 164
DeVol T.A. 173, 187, 240
Didenko K. 122
Dimitriev O.P. 283
Diyuk O.A. 142
Djidjelli H. 196
Dlubovskiy R.M. 228
Dmitruk I. 197
Dmitruk I.M. 157
Dmytruk A. 197
Dmytruk I.M. 131
Dmytrenko O.P. 103
Dmytriv Yu.V. 211
Dobrovolskiy A. 160
Dorbani T. 250
Doronin Yu.S. 258
Doroschuk V. 281
Doroshenko I. 40, 43
Doroshenko I.P. 37, 293
Doroshenko I.Yu. 137
Doroshenko O. 40
Dotsenko I. 116
Dotsenko V.P. 104, 112
Doualan J.-L. 107, 318
Dovbeshko G. 13, 27, 29
Dovhopyatyy Yu. 260
Drozd M. 204
Dryuchko O. 198, 225
Dubey D.K. 323
Dubey I. 30
Dubey L. 30
Dubok V.A. 291
Duca G. 8
Dudok G. 236, 310
Dukarov S.V. 69, 73
Dupliak I. 199, 321
Dusheyko M. 71, 240
Dutka V. 121
Dyachenko A. 200
Dzeryn M. 335
Dzhafarova S.Z. 345
Dzhagan V. 99
Dzhagan V.M. 51
Dzhafarova S.Z. 177
Dziaman I. 236
Dziazko O.G. 201
Dzikovskyi V. 55, 66
Dzundza B. 61
Dzyadevych S.V. 308

E

Efryushina N.P. 112
Eidimtas M. 186
Eken K. 169
Eken S.K. 162, 195
El Haimeur A. 170, 337
Ennan A.A. 228
Ezhova V. 265

F

Fadieiev E.M. 261
Faulques E. 258
Fechan A. 42, 184
Fedchenko A. 202
Fedchenko A.N. 327
Fedorenko G.V. 244
Fedoryak O.M. 283
Fleischer M. 108
Fenping L. 199
Ferenchuk Ye. 14
Fesenko O.M. 96
Fesych I.V. 110, 201, 238
Filatov O.V 54
Filatova V.S. 15
Fitio V. 321
Fomanyuk S.S. 84

Fochuk P.M. 223
Fokin A.A. 72
Fomenko A.S. 203, 255
Fonari M. S. 239

G

Gabchak O.L. 210
Gagolkina Z. 122
Galstian I. 113
Galunov N. 254
Gamernyk R 153
Ganizade G.F. 41
Gaponov A.M. 103
Garashchenko A. 75
Garibova S. N. 50
Gavrilko T. 204, 205
Gayvoronsky V.G. 161, 168
Gelmboldt V.O. 228
Georgiev Y.S. 2
Gerda V.I. 114
Gerush I. 14
Glamazda A. 30
Glazunova V. A. 320
Globa N.I. 77
Glukhov K.E. 227
Glushko E.Ya. 59
Gnatenko Yu.P. 110
Gnatyuk I. 205
Gnatyuk O. 13, 29
Gnilitskyi I. 240
Goleus V. 79
Golovina I. S. 217, 220
Golovynskyi S. 157
Gomeniuk Yu.V. 249
Gomenyuk O. 250
Gomonnai A.V. 51
Gomory A. 305
Goncharenko N.G. 20
Goncharov V.V. 80
Goncharuk O. 200
Gorban O. 124
Gorbyk P.P. 294
Gorishnyi M.P. 96
Gornitsky I. 198, 225
Grankina I. 146
Grazulevicius J.V. 175, 193, 206, 207, 243, 248, 315, 317, 321, 325, 330, 331, 336
Grebenyuk A.G. 111, 115, 145
Gridyakina A. 165
Grigalevicius S. 186, 323
Grishchenko L.N. 203, 255
Gruodyte A. 175
Grygorova G. 277, 309
Grygorova G.V. 284
Gryn D.V. 16, 37
Grynko D. 188
Grytsenko O. 184
Gryshchouk G. 153
Grytsenko K. 339, 341
Gubanov V. 5, 12, 98, 116
Gubriy Z.V. 45
Gudeika D. 137, 207, 243, 317, 331
Gudyma Iu. 208
Gudimenko V.A. 215
Gudymenko O. 249
Gumienna-Kontecka E. 36
Guozhu Y. 199
Gura S. 192
Gurova Yu. 17
Guryn P.O. 15
Guzauskas M. 248, 336
Guzenko N.V. 210
Gvozdovskyy I.A. 160, 211

H

Hajiali A. 212
Hajiyeva F.V. 159
Halechko H. 121
Hamamda S. 250
Hanulia T. 27
Harbuz D.O. 215
Havryliuk O.O. 106
Herus A.O. 258

Hodlevska M. 216
Hodlevskyi M. 216
Horbatenko Yu.V. 322
Horbenko Yu. 335
Horbenko Yu.Yu. 138, 320
Horiunova I. 279
Hrabovsky E. 197
Hrytsko H. 235
Hsueh T.-C. 323
Hubenko K. 297
Hubenko K.O. 285, 312
Hura A.O. 246
Huseynova A.S. 159
Husson S.M. 187

I

Iarova N. 178
Ibragimov T.D. 41
Ibrayev N.Kh. 143, 155, 176
Idres C. 276
Idrissi A. 32
Ilchenko M. 30
Ilchuk H. 55, 66, 78
Ilnytskyi Y. 42
Ilyin P.P. 97, 100
Imamaliyev A.R. 41
Imamaliyeva S.Z. 209, 268
Isayev A.I. 7, 50, 93
Isaeva O. 99
Ischenko O. 200
Ishchenko A.A. 143, 176, 187, 221
Ishkov Yu.V. 228
Ismailova E.N 219
Iukhymenko N. 65, 182, 242
Ivanytska I. 198, 225
Ivakh M.S. 18
Ivakha N. 329
Ivanenko I. 202, 234
Ivanitska V.G. 223
Ivaniuk Kh. 321
Ivaniuk K. 199, 206, 256
Ivaniuk H.B. 320
Ivanov O.V. 201
Ivanov V.V. 32, 117
Ivashchyshyn F. 156

J

Jeżowski A. 322
Jou J.-H. 323

K

Kachkovsky A. 12
Kachkovsky O. D. 26, 131
Kadan V. 169
Kadashchuk A. 6, 152, 333
Kachmar A. 216
Kaci M. 276
Kalchenko V.I. 68
Kaleinikova O. 278
Kalugin O.N. 32
Kamarchuk G.V. 215, 222, 258
Kamarchuk L.V. 222
Kanak L.M. 223
Kanchev K.S. 2
Kanyuk M.I. 22
Kapush O. 279
Karachevtsev V. 30
Karbovnyk I.D. 138
Karpenko O.S. 111, 118
Karpenko S. 75
Karpenko Yu.V. 224
Karpicz R. 205, 254
Kartel M.T. 118, 289
Kartel N.T. 111
Karvatskiy I. 278
Kasatkin A.L. 88
Kashuba A. 55, 66, 78
Kavetskyy T 151
Kavok N.S. 277, 285
Kazantseva Z.I. 68, 160
Keda T.Ie. 74

Kenaz R. 108
Kerita O. 254
Keruckas J. 325
Keruckiene R. 206
Kettouche H. S. 213
Khabuseva S. 21
Khaniukov V. 198, 225
Kharchenko O. 164, 226
Kharchenko T.O. 286, 306
Kharkhalis L.Yu. 227
Khatsevich O.M. 272
Khilya O.V. 74
Khlebnikova M.E. 104, 112
Khodzhaieva R.S. 19
Khoma R.E. 228
Khomenko A.V. 20, 23, 25
Khomenko O.V. 104, 112
Khomenkova L.Yu. 252
Khomyak S.V. 45
Khristenko I.V. 117
Khrypunova A.L. 69
Khrypunova I.V. 73
Khyzhun O. 249
Kinzhybalo V. 256
Kiose T.A. 267
Kirichenko M.V. 73
Kisyl D. 249
Kitova S. 2
Klenina O. 287
Klepikova K.S. 69, 73
Klepko V. 326
Klepko V.V. 203, 255
Klishevich G.V. 141
Klochko N.P. 69, 73
Klochkov V. 277
Klochkov V.K. 284, 285, 312
Klymchuk D.O. 203, 255
Kniazieva K.S. 45
Kobzev D. 21
Koci K. 262
Köhler A. 152
Koksharova T.V. 229, 241
Kołacińska K. 173
Kolbasov G.Ya. 75, 84
Koledov V.V. 144
Kolendo A.Yu. 161, 168, 242, 270
Kolesnik V. M. 133
Kolosova O. 21
Komarenko D. 161
Kondratenko O. 271
Kondratenko O.S. 60, 328
Kondratenko S. 52
Konopelnyk O.I. 119
Konotop A.P. 215
Kopach V.R. 69, 73
Kopčanský P. 47
Korenivski V. 64
Kornienko N.E. 5, 11, 98, 101
Kornii A. 70
Kornii Y. 230
Korobeinyk A.V. 231
Korobsky V.V. 245
Korolyuk O.A. 322
Korostil A.M. 166
Korsunska N.O. 252
Kosevich M. 305
Koshets I.A. 68
Kosogina I. 202
Kostetskyi A.O. 120
Kosyanchuk L. 232
Kosyanchuk L.F. 105, 141
Kotova N.V. 328
Kotsun V. 42
Kotsyubynsky V. 216
Koval V.M. 71
Kovalchuk O.V. 47, 48
Kovalchuk S.I. 288
Kovalenko M. 55, 66
Kovalenko S.I. 33
Kovalenko S.M. 32
Kovalska V. 36, 296
Kovalskyi Ya. 121
Kowalonek J. 164
Kozak N. 122, 232
Kozak N.V. 178
Kozakevych R.B. 233
Kozanecka-Szmigiel A. 164
Kozoriz K. 318
Kozyreva T. 79
Kramar O. 260

Krasinskyi V. 263
Kravchenko A.V. 222
Kravchenko I. 274
Kravchenko T.V. 246
Kravchenko V.V. 62, 87
Kravchuk R. 160
Kravets A.F. 64
Kravtsov V. Ch. 239
Kremer I.P. 18
Krivchikov A. I. 322
Krivets O.S. 171
Krivoruchko Ya.S. 344
Kromka A. 174
Krucaite G. 186, 323
Kruglenko I. 319
Kruglyak O. 257
Krupa M.M. 166
Krupka O. 164, 226
Krupskaya T.V. 289
Krysa B.V. 290
Krysa V. M. 290, 301
Kryshenik V.M. 51
Kublanovsky V. 89
Kublanovsky V.S. 77
Kudrya V.Yu. 157
Kukh A. 234
Kukhta N. 206
Kukla O. 139
Kukla O.L. 324, 327
Kulai I. 168
Kulikov L.V. 11
Kulikova O. 4, 239
Kulish M. 134
Kulish M. P. 22, 97, 100, 103
Kunitskaya L. 326
Kuranda N.N. 87
Kurnosov V. 124
Kurochka L.I. 100
Kurta S. A. 272
Kusyak A.P. 294
Kusyak N.V. 291, 294
Kutsevol N. 123, 235, 274, 278, 280, 281, 292, 298, 301, 303
Kutsiy S. 256
Kuziv Yu.I. 235, 378, 380, 292
Kychkyruk O. 273, 332
Kyrychenko A.V. 17, 32
Kysil A. I. 170, 327
Kysil Kh. 236
Kytaihora K. 198, 225

L

Labbé C. 318
Lamkiewicz J. 34
Lamonova K. 124
Lazarenko M. 52, 250
Lazarenko O. 125
Lazarev I. 254
Lazoryk I.V. 126
Le Normand F. 147
Lebedev V. 237
Lebedyeva I. 10
Lelyushok S. 281
Lemishko S. V. 217, 220
Len E. 113
Len E.G. 127
Len T. A. 132, 147
Len T. S. 127
Lendel V.V. 201
Lopatina Ya.Yu. 72
Leonenko E. 151
Leonov V.O. 128
Lesiuk A.I. 22
Levchenko G.G. 238
Levchyk V.M. 91
Levkov I.V. 170, 337
Liakh M.V. 227
Liakvovetskyi V.R. 167
Liaskovska M. 295
Liedienov N.A. 238
Lin W.K. 330
Lisetski L.N. 211
Lisnyak V.V. 70
Lizunov V. V. 127
Lobanov V.V. 334
Logvinenko D.T. 23
Lokshyn M. 307
Luchynets M.M. 47

Lopatynskyi A.M. 22
Lopushanska B.V. 129
Lopushansky V.V. 51, 129
Losytskyy M. 40
Losytskyy M.Y. 137, 293, 296
Loya V.Y. 51
Lozovan V. N. 239
Lozovski V. 307
Lozitsky O.V. 130, 132
Lunko T.S. 60, 328
Lutsenko L.V. 244
Lutsyk P.M. 120
Lysenko V. 307
Lytvyn R. 256
Lytvynenko A. 278
Lytvynenko Ya.M. 64
Lyubov V.M. 73

M

Magunov I. 90
Maiko K.O. 131
Makeeva I. M. 133
Makeiev A.M. 74
Maksimchuk P. 124, 154, 297, 304, 309
Maksimchuk P.O. 285, 312
Maksymov A. 208
Maksymovych N.P. 244, 247
Maksymych V. 156
Malek M 325
Malynovskyi M. B. 44
Malyukin Yu. 124, 140, 146, 154, 297, 304, 309
Malyukin Yu.V. 284, 285, 312
Maltseva T. 89
Mammadova A.T. 209
Mammadova H.I. 7
Mamontova I.B. 60, 328
Mamunya Ye. 134
Mamykin S.V. 60, 63, 67, 240, 328
Mamykin A.V. 139, 324
Mandzii T.V. 229, 241
Manousaki A. 52
Marchenko A.A. 72
Markovsky B. 57
Marton M. 174
Martynes-Harsiia A. 242
Martynyuk V. 298, 303
Marynin A.I. 269
Mashadiyeva L.F. 181, 219
Masimukku N. 243
Mateychenko P.V. 215
Matkivska G. M. 320
Matushko I.P. 244, 247
Mazna Yu.I. 38
Mazur N. 99
Mazur T. 61
Matzui L. 125
Matzui L.Yu. 130, 132, 147, 148
Medyk I. 75
Mekhtiyeva S.I. 7, 50, 93
Melekhovets O. 286, 299, 306
Melekhovets Y. 286, 299, 306
Melikova S.Z. 177
Melnic E. 4
Melnik N. 235
Melnyk D. O. 24
Melnyk O. Ja. 24
Melnyk V.I. 141
Melnyk Yu. 310
Merzhyievskyi D.O. 131
Miannay F.-A. 32
Milekhin I. 108
Milokhov D.S. 74
Mishura V. 299
Misiura A. 134
Mocreac O. 86
Mokrinskaya E.V. 62, 87, 221
Mosendz A.O. 91
Mozkova O. 90
Mrachkovska N. 300
Mrachkovsky A.M. 245
Mukha Yu. 307
Multian V. 161, 168
Musina A.O. 246
Myagchenko Yu. 43
Myhalchuk A.O. 340
Mykhailova H.Yu. 135
Mykytyuk Z.M. 18, 45
Myronyuk I. 139

N

Nadtoka O. 97, 281, 298, 301, 303
Nagorna T.V. 136
Nalyvaiko V. 300
Naoui Y. 250
Nasiri S. 315
Nasser H. 189, 343
Narbutaitis E. 248
Naumenko A.P. 5, 11, 12, 98, 101, 116, 123, 137, 279
Navozenko A. 12
Navozenko O.M. 137, 341
Nazar A.P. 267
Nazarov A. 249
Nazarov A.N. 67
Nazarova T. 249
Nedilko S.A. 201
Nedilko S.G. 52, 250
Negriyko A.M. 105
Nesin S. 122
Nessin S. 326
Nikitchuk O. 263
Nikitenko V.M. 77
Nikolaeva O.A. 269, 271, 293
Nikolaiev R.O. 251
Nikolenko A. 27, 29
Nicorici V. 76
Nosenko V. 318
Nosenko V.V. 252
Noskov Yu. 139, 173

O

Obernikhina N.V. 26, 131
Oblovatna S. 75
Obukhova O. 21
Obushak M. 256
Ogurtsov N. 139, 257
Ogurtsov N.A. 173, 324
Ogurtsov V. 287
Ohulchanskyy T.Y. 37, 269, 293, 302
Okovytyy S. I. 33
Okrushko E. 304, 309
Okulov S.M. 252
Okushko O. 300
Oleksenko L.P. 244, 247
Olenchuk M. 27
Olenych I.B. 138
Olenych Yu.I. 138
Oliinyk Y. 28
Oliynyk V. 257
Oliynyk V.V. 130
Omastova M. 134
Omielaieva V. 297
Onanko A.P. 97, 100, 103
Onanko Y.A. 97, 100
Oranska O.I. 210
Orel S. 124
Orujlu E.N. 253
Ostapenko N. 254
Ostapenko Yu. 254
Ovdenko V. 161, 168, 218, 221
Ovsiienko I. V. 147

P

Pak V. 299
Paluszkiewicz C. 29
Panasenko A. I. 224
Pancheva H. 259
Papadopoulos A. 52
Pashazadeh R. 206
Pavlenko V. 235
Pavlov E. 3
Pavlov I. 160, 169, 189, 195, 343
Pavlov V. 62, 87, 218, 221
Pavlova S. 169, 195
Pavlusiak N. 249
Pashchenko A.V. 238
Pashkevich Yu. 124
Pashynska V. 305
Patoka V. I. 133
Pavlenko O.L. 22, 97, 100
Pavlenko T.V. 83

Perederii O. 27
Permyakova N.M. 203, 255
Persson B.N.J. 23, 25
Petkov V.D. 2
Petranovska A.L. 294
Petrina R.O. 18, 45
Petrov E.G. 128
Petrovska H. 321
Petrus R. 55, 66, 78
Petrushenko S.I. 69, 73
Petrychuk M. 257
Petryk I. 262
Piergies N. 29
Pilipenko A. 192, 259
Pinchuk-Rugal T.M. 22, 97, 100, 103
Piryatinski Yu.P. 44, 120, 131
Pitkovych Kh. 256
Pliusnina M. 4
Plokhovska S. 279
Poberezhets S.I. 47
Podust G. 40, 293
Pogodin A.I. 47
Pogorelov O.E. 54
Pogrebnyak V.G. 238
Pokhodylo N. 256
Poletaev N.I. 104, 112
Polishchuk D.M. 64
Polishchuk V. 313
Polupan Ya. 254
Polyshchuk L.M. 233
Popovych D.I. 126
Pospelov A.P. 215, 222, 258
Powell B.A. 173
Prochazka M. 134
Prokopets V. 250
Prokopiv M. M. 217
Prokopiv V. 61
Prostota Ya.O. 131
Prystai T.V. 18
Pud A.A. 139, 173, 257, 324
Pundyk I.P. 22
Pylypenko A. 134
Pylypenko O. O. 33

Q

Qu J. 157

R

Rabiy V.I. 119
Rachkov A. 107
Radchenko T.M. 150
Radfar B. 189
Radko A.S. 286, 306
Radko I. 300
Raievska O. 99
Rakitskaya T.L. 267
Ramazanov M.A. 159
Rapaport R. 108
Rashevska A. 35
Rawiso M. 292
Revo S. 250
Ripko O.P. 247
Rogovtsov O.O. 83
Romanov M.D. 215
Romanova E. 31
Romantsova O.O. 322
Romanyuk V.R. 60
Ropakova I. 140
Roshal A.D. 17, 19
Roshchin O.M. 141
Rozhin A. 120
Rozhkovskiy O.M. 97
Rud M. 113
Rudenko V.I. 167
Rudnichenko A.V. 211
Rusakova N.V. 261
Rusavsky A. 249
Rusavsky A.V. 67
Rusetskii I.A. 84
Rusinchuk N. 307
Ryazanova O. 30
Rybak A. 160

S

Sachuk O.V. 142
Sadykova A.E. 155
Saenko G. V. 147
Saiapina O.Y. 308
Salei An. 79
Salman S.H. 162
Sanzhak O.V. 80
Savchenko I.O. 271, 273, 329, 332, 338
Savchenko O. 229, 241
Savytskyi A.V. 258
Scherbatskii V. 52, 250
Scolyar G.I. 247
Seliman A.F. 187
Seliverstova E.V. 143
Selyshchev O. 99
Semchuk O.Yu. 106
Semenova O. 21
Semenyuk N. 236, 310
Seminko V. 124, 154, 297, 304, 309
Semikina T.V. 63, 67
Semkiv I. 55, 66, 78
Serdiuk I.E. 19
Serednytski A.S. 126
Sergeieva T. 33
Shablykin O. 131, 230
Shapovalov V.A. 144
Shapovalov V. V. 144
Sharanov I.P. 283
Shatnii T. D. 127
Shavrov V.G. 144
Shcherbakov O.B. 293
Shcherban N. 204
Shcherban N.D. 205
Sheludko V. 250
Shembel E. 57
Shevelkov A.V 219
Shevchenko Ye.V. 128
Shirshov Yu.M. 327
Shkolnikova T. 259
Shmatok Yu.V. 77
Shmeleva L. V. 102
Shmyryeva L.N. 63
Shukurova G.M. 181
Shyrchenko D. 226
Shyshchak O. 81, 180
Sihunov O.O. 246
Silchenko D. 259
Simokaitiene J. 193, 206, 325, 336
Sini G. 193
Siniugina A.T. 82
Skhirtladze L. 330
Skorenkyy Yu. 260
Skorobahatko M.V. 211
Skorokhoda V. 236, 310
Skowroński Ł. 164
Skuodis E. 206, 331
Slisenko O. 182, 265
Sliusarchuk L.I. 83
Slobodian O. 249
Slominskii Yu.L. 137, 283, 341
Smertenko P. 151
Smilyk V.O. 84
Smirnova O.V. 145
Smokal V. 164, 226
Smola S.S. 261
Snegurskaya T. 31
Snegursky A. 31
Snopok B. 319
Solonenko D. 51, 129
Solopan S. O. 220
Song C. 238
Sorokin A. 140, 146
Spodoba M.O. 311
Spylka D. O. 147
Sribna V. 278
Stakhira P. 206, 256, 321
Stanicka M. 256
Stankevich A. 333
Stanoeva N.A. 2
Stanovyi O. 197
Styopkin V.I. 167, 204
Stara T. 318
Starukh H. 262
Starykov G.O. 320
Stashkiv O. 153
Stepanenko O. 21
Stepanenko Ye.Yu. 46, 251
Stepaniuk D.S. 32

Stepanov V. 249
Sternik D. 271, 273, 332
Storozhenko D. 198, 225
Stoianov Yu. 109
Strizhak P. 151
Stroyuk O. 99
Studenyak I.P. 47, 129
Studzinsky S.L. 62, 82, 85, 87, 114
Styopkin V. 165
Sviatenko L. K. 33
Suberlyak O. 184, 263
Sukhov V.M. 69
Suprun A.D. 102
Surovtseva E.R. 327
Sutkuviene S. 186
Swayamprabha S.S. 323
Sych G. 315, 336
Syromiatnikov V. 270
Syrotynska I. 34
Sytnik O. 299
Syvolozhskyi O. A. 125, 148
Szewczyk D. 322
Szmigiel D. 164

T

Tagare J. 323
Tagiyev M.M. 94, 149, 177
Tamuliene E. 31
Tan X. 206
Tananaiko O. 70
Tang J. 108
Tarasenko S. 311
Tatarchuk T. 295
Tatarenko V.A. 150
Tatarets A. 21
Tavgeniene D. 186
Telbiz G. 151
Temirbayeva D.A. 143
Terebinska M.I. 334
Terentyeva Yu. 35
Tereshchenko O. 43
Tertykh V.A. 231, 233
Teselko P. 52, 197, 250
Teselko P.O. 157
Timko M. 47
Tkach V.I. 144
Tkachuk O.I. 334
Tkachuk Z.U. 16
Tkachuk Z. Yu. 46, 251
Tokar A.V. 264
Tolstov A. 265
Tolstov O. 182
Tomchuk A.V. 157
Tomkeviciene A. 206, 256
Tovstenko-Zabelin M. 271
Tovstolytkin A.I. 64
Trepachko M. 217
Tretyakova I.M. 296
Truba A.S. 267
Trunova E.K. 329
Trunova O.K. 83, 338
Tsapko E. 113
Tsaregradskaya T. L. 147
Tsiulyanu D. 58, 86
Tsizh B. 335
Tsupryk H. 109
Tsvitkovskyi V.P. 88
Tsyba M.M. 142
Tunçkol E. 195
Tupychak M. 256
Turan R. 189
Türker V. 162, 195
Turkov O.V. 132
Turov V.V. 289
Tykhomyrova T. 237

U

Uklein A. 168
Ukrainets N. 78
Ukraintsev E. 174
Urbonas E. 256
Ushakov M. V. 127

V

Vaidyanathan S. 323
Vahula O.A. 327
Vakarov S. 36
Vakhnin A. 152, 333
Vakula V.L. 258
Valkunas L. 254
Vartik P. 43
Vashchenko O.V. 280
Vasilev A. 2
Vasilieva A.V. 117
Vasin A. 249
Vasin A.V. 67
Vasylechko V. 153
Vasylyev M.O. 15, 133
Veligina E. S. 26
Venhryn Yu.I. 126
Verbitsky A.B. 120
Viagin O. 124, 154
Vicol C. 8
Videva V. 2
Viduta L. 165
Vilchinskyi V.V. 148
Vinogradova-Anyk O. 278
Virsta T. 121
Virych Pavlo 298, 301, 303
Virych Petro 303
Vistak M. 320
Vityuk N. 307
Vlasenko N. 151
Vodzinskiy S.V. 228
Voitenko T.A. 201
Voitenko Z.V. 170, 337
Vojs M. 174
Volchak G. 90
Volkova G. 124
Volkova V.Y. 267
Voloshin I. 30
Voloshin Y. 36
Volovenko Yu.M. 74
Volyniuk D. 175, 193, 206, 207, 243, 248,256, 315, 321, 331, 336
Vorobets V. 75
Vorona I. 318
Vorona I.P. 220, 252
Vovchenko L.L. 130, 132, 148
Vovk M. V. 211
Vovk V.E. 48
Voynarovych I.M. 51
Voznesenskaya T. 278
Vretik L. 203, 255, 269, 271, 293, 332
Vukstich V. 31
Vyshnevsky D. 218, 221, 270

W

Wårgberg T. 174
Wojkiewicz J.-L. 139

X

Xue B. 157

Y

Yadav R.A.K. 323
Yağcı E. 169
Yağcı M.E. 162, 195
Yakovenko O.S. 148
Yakovyna V. 42
Yakubiak M.R. 272
Yanovska E. 271, 273, 332
Yapontseva Yu. 89
Yashchenko O. 52
Yashchenko O.V. 69
Yashchuk V.M. 3, 10, 16, 37, 40, 46, 137, 293
Yefimova S.L. 140, 146, 284, 285, 297, 312
Yegorova T. V. 170, 337
Yeremenko A.V. 222
Yeshchenko O. 197
Yeshchenko O.A. 157

Yuchen L. 199
Yukhymchuk V. O. 220
Yushchenko O.V. 171

Z

Zablodskiy M.M. 282, 288, 311
Zagorodnii V. 257
Zagorodnii V.V. 130
Zagorodnya S. 307
Zahn D. 108
Zahn D.R.T. 51, 99, 129
Zakharov M.V. 25
Zapukhlyak R. 216
Zazhigalov V.A. 80, 142
Zelenko M.A. 201
Zelentsov V. 194
Zelinskiy A. 153
Zembouai I. 276
Zeynalova G.S. 209
Zimenkovsky B. 287
Zinchenko O. 265
Zinchenko V. 90
Ziółkowska D. 34
Zhadan D.O. 69, 73
Zhang B. 186
Zheleznova L.I. 83
Zheltonozhskaya T. 203, 255, 326
Zhugayevych A. 152
Zhuk T.S. 72
Zhumabekov A.Zh. 155
Zhuravkov O. 125
Zolfaghari Borra M. 189, 343
Zorin V. 123, 274, 292
Zorina T. 274
Zubrevicius R. 331
Zui M.F. 91
Zuy O.V. 38

CONTENTS

SECTION 1. Electronic processes at interfaces of organic materials with metals, as well as biological, organic, and inorganic media

ANALOGUES OF THIAZOLE ORANGE – NEW SYNTHETIC CONDITIONS AND PHOTOPHYSICAL PROPERTIES OF LIPOPHILIC ASSYMETRIC MONOMERIC MONOMETHINE CYANINE DYES – NONCOVALENT NUCLEIC ACIDS BINDERS 2
V. Videva, A. Vasilev, S Kitova, Y. S. Georgiev, K. S. Kanchev, N. Al. Stanoeva, V. D. Petkov

NESTED MAPPING FOR DECONVOLUTION AND FUNCTION TRANSITION 3
Eugen Pavlov, Valeriy Yashchuk

PHOTOLUMINESCENCE PROPERTIES OF SIX NEW METAL-ORGANIC COMPOUNDS WITH 4,4-DIAMINODIPHENYLMETHANE LIGAND 4
O. Kulikova,V.Cociu, M.Pliusnina, E.Melnic, L. Croitor, D. Chisca

ANTISTOKS AND STOKS RAMAN SCATTERING IN MOLYBDENUM DISULPHIDE (MoS_2) AND GRAPHENE UNDER EXCITATION BY CONTINUOUS LASER RADIATION 5
Kornienko N.E., Naumenko A.P., Gubanov V.O.

DETERMINATION OF THE DENSITY-OF-STATES IN OLED ORGANIC SEMICONDUCTORS USING THERMALLY STIMULATED LUMINESCENCE 6
Andrey Kadashchuk

THE STUDY OF THE CHARACTERISTICS I – V FOR THE CHALCOGENIDE GLASS COMPOSITIONS WITH SANDWICH STURUCTURE $Te\text{-}Ge_{8.33}As_{16.67}Te_{75}\text{-}Al$, $Te\text{-}Ge_{10}As_{20}Te_{70}\text{-}Al$ AND $Te\text{-}Ge_{12.5}As_{25}Te_{62.5}\text{-}Al$ 7
A.I. Isayev, S.I. Mekhtiyeva, H.I. Mammadova

THE INFLUENCE OF TARTARIC ACID ON DPPH RADICAL SCAVENGING ACTIVITY OF VITAMIN C 8
Crina Vicol, Gheorghe Duca

SOLITON FACILITATED LONG-RANGE ELECTRON TRANSPORT IN DONOR-POLYMER-ACCEPTOR SYSTEM 9
Larissa Brizhik

INFLUENCE OF SPATIAL STATIC AND DYNAMIC INHOMOGENEITIES ON THE DISTRIBUTION OF ELECTROELASTIC FIELDS AND ELECTRONIC PROCESSES IN PIEZOCERAMIC COMPOSITES 10
I. Lebedyeva, V. Yashchuk, O. Boryseiko

OBSERVATION OF GRAPHENE- AND DIAMOND-LIKE NANOSTRUCTURES IN MoS_2-BASEDCOMPOSITES WITH SMALL CARBON ADDITIVES 11
Kornienko N.E., Naumenko A.P., Kulikov L.M.

ORGANIC DYE GRAPHENE HYBRID STRUCTURES: AN AB INITIO STUDY 12
A. Navozenko, A. Naumenko, V. Gubanov, A. Kachkovsky

COHERENT ANTI-STOKES RAMAN SCATTERING SPECTROSCOPY AND IMAGING OF DNA ON GRAPHENE LAYERS 13
Galyna Dovbeshko , Olena Gnatyuk , Andrej Dementjev

ELECTRON TRANSPORT CHAIN IN THE LIVER BY KIDNEY DISEASE
Ferenchuk Ye., Bevzo V., Gerush I. 14

CHANGE OF ELECTROCHEMICAL POTENTIALS FOR DENTAL IMPLANTS SURFACE IN A PHYSIOLOGICAL SOLUTION
M.O. Vasylyev, V.S. Filatova, P.O. Guryn 15

SOME PECULIARITIES OF SPECTRAL PROPERTIES OF VARIOUS COMPOUNDS OF ADENINE NUCLEOTIDE AND POLYNUCLEOTIDE
Gryn D.V., Yashchuk V.M., Tkachuk Z.U. 16

COMPLEX FORMATION OF o-POPOP WITH THE ALKALINE EARTH METAL IONS IN ACETONITRILE SOLUTION: DFT AND MOLECULAR DYNAMICS SIMULATION STUDIES
Yuliia O. Gurova, Alexander D. Roshal, Alexander V. Kyrychenko 17

OPTICAL SENSOR FOR DETECTING THE AMINO ACIDS CONCENTRATION IN AQUEOUS SOLUTIONS
Mykytyuk Z.M., , Barylo H.I., Petrina R.O., Kremer I.P., Ivakh M.S., Prystai T.V. 18

8-FORMYL-7-HYDROXYFLAVONE AS ION SENSOR. COMPLEX FORMATION WITH Mg^{2+} IONS
Ruslana S. Khodzhaieva, Ilia E. Serdiuk, Alexander D. Roshal 19

COMPUTER MODELING OF FRICTION OF ULTRATHIN LAYER OF CARBON DISULFIDE CONFINED BETWEEN DIAMOND SURFACES
A.V. Khomenko, D.V. Boyko, N.G. Goncharenko 20

INFLUENCE OF HEAVY HALOGEN ATOMS ON SPECTRAL PROPERTIES AND QUANTUM YIELDS OF HEPTAMETHINE CYANINE DYES
D. Kobzev, O. Semenova, O. Obukhova, S. Khabuseva, O. Kolosova, O. Stepanenko, A. Tatarets 21

MECHANISMS OF THE INTERACTION OF BOVINE SERUM ALBUMIN WITH GEMCITABINE
A.I. Lesiuk, O.P. Dmytrenko, T.O. Busko, O.L. Pavlenko, I.P. Pundyk, T.M. Pinchuk-Rugal, M. P. Kulish, Chegel V.I., A.M. Lopatynskyi, Kanyuk M.I., L.V. Denis 22

STATISTICAL REPRESENTATION OF SELF-SIMILAR MODE OF ICE SURFACE PREMELTING DURING FRICTION
A.V. Khomenko[a], D.T. Logvinenko, B.N.J. Persson 23

REASONS FOR CHANGING THE ABSORPTION SPECTRUM IN THE ASSOCIATION OF NEW METHYLENE BLUE WITH SURFACTANTS
Melnyk D. O., Melnyk O. Ja. 24

MOLECULAR DYNAMICS OF FRICTION OF METAL NANOPARTICLES ADSORBED ON GRAPHENE SHEET
A.V. Khomenko[a,b], M.V. Zakharov[a], B.N.J. Persson 25

ENERGY OF THE ROTATION BARRIERS PHENYL SUBSTITUENTS IN PYRAZOLO[1,5-*a*][1,3,5]TRIAZINES AS A FACTOR THE STABILIZATION OF [PHARMACOPHORE-BIOMOLECULE] COMPLEX 26

E. S. Veligina, N. V. Obernikhina, O. D. Kachkovsky, V. S. Brovarets
ENHANCED DNA RAMAN MODES PROBED BY SiO_2 PHOTONIC CRYSTALS
M. Olenchuk, T. Hanulia, O. Perederii, A. Nikolenko, G. Dovbeshko 27
DEVELOPMENT OF AN EFFECTIVE METHOD OF MANURE CLEANING ON PIG COMPLEXES USING HIGH-VOLTAGE ELECTRIC-PULSE EQUIPMENT 28
A. Chmil, Y. Oliinyk
INFRARED AND CARS SPECTROSCOPY STUDY OF MITOCHONDRIA
I. Polovyi, N. Piergies, C. Paluszkiewicz, A. Dementjev, O. Gnatyuk, A. Nikolenko, G. Dovbeshko 29
SELF-ASSEMBLED PORPHYRIN AGGREGATES ON BIOPOLYMER SURFACE AS A PLATFORM FOR LIGHT HARVESTING AND ENERGY TRANSFER
O. Ryazanova, I. Voloshin, A. Glamazda, L. Dubey, M. Ilchenko, I. Dubey, V. Karachevtsev 30
HIGH- AND LOW- ENERGY IONIZING RADIATION EFFECT ON THE BIOLOGICALLY RELEVANT AMINO ACID VALINE MOLECULE 31
A. Snegursky, E. Tamuliene, V. Vukstich, T. Snegurskaya, E. Romanova
COUMARIN BASED DONOR-ACCEPTOR DYES FOR DYE-SENSITIZED SOLAR CELLS. THEORETICAL INVESTIGATION
Stepaniuk D.S., Blazhynska M.M., Kalugin O.N., Kovalenko S.M., Kyrychenko A.V., Miannay F.-A., Idrissi A., Ivanov V.V. 32
ELECTRONIC PROPERTIES OF 1,2,4-TRIAZOLE DERIVATIVES: A DFT STUDY 33
O. O. Pylypenko, S. I. Okovytyy, L. K. Sviatenko, T. Sergeieva, S. I. Kovalenko
FORMATION OF ION ASSOCIATES IN THE CARRAGEENAN - PINACYANOL SYSTEM 34
Iryna Syrotynska, Dorota Ziółkowska, Jan Lamkiewicz
TOWARDS THE UNDERSTANDING OF NAD(H) COENZYME FLUORESCENCE AT AMBIENT CONDITIONS 35
Yuliya Terentyeva[a], Anastasiia Rashevska
CD SENSITIVITY OF THE MONO-CARBOXYPHENYLSULFIDE IRON(II) CLATHROCHELATES TO GLOBULAR PROTEINS 36
N. Chornenka, S. Vakarov, E. Gumienna-Kontecka, Y. Voloshin, V Kovalska
THE SPECTRAL MANIFESTATIONS OF INTERACTION BETWEEN DNA AND METAL IONS 37
Gryn D.V., Yashchuk V.M., Ohulchanskyy T.Y., Doroshenko I.P.
COMPARISON OF SORBENTS FOR THE REMOVAL OF ORGANIC COMPOUNDS THAT INTERFERE WITH THE DETERMINATION OF BROMIDE IONS IN NATURAL WATERS 38
O.V. Zuy, Yu.I. Mazna

SECTION 2. Electro-optic processes in liquid-crystal-based heterogeneous systems

SPECTROSCOPIC STUDY OF SELF-ASSEMBLING PROCESSES IN AQUEOUS SOLUTIONS OF LYOTROPIC LIQUID CRYSTALS 40

I. Doroshenko, G. Podust, V. Degoda, M. Losytskyy, V. M. Yashchuk, O. Doroshenko, V. Balevicius

DIELECTRIC RELAXATION AND ELECTROOPTIC EFFECTS IN FULLERENES-DOPED NEMATIC LIQUID CRYSTALS 41
T.D.Ibragimov, A.R.Imamaliyev, G.F.Ganizade

DYNAMIC CHARACTERISTICS OF THE ELECTRICALLY DRIVEN LIQUID CRYSTAL PLANARS LIGHT GUIDE 42
O. Chaban, A. Fechan, Y. Ilnytskyi, V. Kotsun, V. Yakovyna

SPECTROPHOTOMETRIC STUDY OF RELATIVE CONTENT OF FLAVONOIDS IN NATURAL OBJECTS 43
Yu. Myagchenko, O. Tereshchenko, P.Vartik, I. Doroshenko

INFLUENCE OF MEROCYANINE DYE AGGREGATION ON SINGLE AND DOUBLE-PHOTON EXCITATION OF FLUORESCENCE IN A LIQUID CRYSTAL TEMPLATE 44
M. B. Malynovskyi, Yu. P. Piryatinski

IDENTIFICATION AMINO ACIDS IN CALLUS BIOMASS OF PLANTS BY OPTICAL SENSOR 45
Petrina R.O., Khomyak S.V., Gubriy Z.V., Kniazieva K.S., Mykytyuk Z.M.

SPECTRAL STUDIES OF THE COMPLEX OF ADENOSINE MONOPHOSPHATE AND D-MANNITOL 46
Ye. Yu. Stepanenko, V.M.Yashchuk, Z. Yu. Tkachuk

ELECTRICAL CONDUCTIVITY OF COMPOSITES BASED ON 6CB LIQUID CRYSTAL AND $(Cu_6PS_5I)_{0.5}(Cu_7PS_6)_{0.5}$ SUPERIONIC NANOPARTICLES 47
I.P. Studenyak, O.V. Kovalchuk, S.I. Poberezhets, M.M. Luchynets, A.I. Pogodin, M. Timko, P. Kopčanský

INFLUENCE OF LIGHT ON THE DIELECTRIC PROPERTIES OF A MIXTURE OF NEMATIC LIQUID CRYSTAL WITH C60 FULLERENE IMPURITIES AND MOLECULAR COMPLEXES Ni-TMTAA-TCNQ 48
Vovk V.E., Kovalchuk O.V.

SECTION 3. Thin film structures and their application

LOCAL STRUCTURE OF $Se_{95}As_5(EuF_3)_1$, $Se_{95}Te_5(Sm)_1$ AND $Ge_{20}Sb_{20.5}Te_{51}$ CHALCOGENIDE GLASSY SEMICONDUCTOR SYSTEMS 50
S. N. Garibova, A.I.Isayev, S.I. Mekhtiyeva, S.U. Atayeva

STRUCTURAL AND SPECTROSCOPIC CHARACTERISATION OF As–Se–S:Cd FILMS 51
Y.M. Azhniuk, V.M. Dzhagan, D. Solonenko, V.V. Lopushansky, V.Y. Loya, V.M. Kryshenik, I.M. Voynarovych, A.V. Gomonnai, D.R.T. Zahn

INFLUENCE OF ORGANIC AND INORGANIC ADDITIVES ON THE PROPERTIES OF NANOCELLULOSE MATERIALS 52
V. Barbash, O. Yashchenko, O. Alekseev, S. Kondratenko, M. Lazarenko, S.G. Nedilko, V. Scherbatskii, P. Teselko, M. Androulidaki, A. Manousaki, A. Papadopoulos

ELLIPSOMETRY OF NANOSTRUCTURED LAYERS 53
E. Bortchagovsky

ELECTROPHYSICAL PROPERTIES CARBON-DOPED THIN FILM IRON
V.O. Burlakov, O. V Filatov, O.E. Pogorelov 54

OPTICAL FUNCTIONS of HEAVY DOPED ZnO:Al THIN FILMS
V. Dzikovskyi, O. Bovgyra, M. Kovalenko, A. Kashuba, H. Ilchuk, R. Petrus, I. Semkiv 55

ABSORPTION SPECTRA OF A LAYER OF METALLIC ELLIPSOIDAL NANOPARTICLES ON A SURFACE SUPPORTING SURFACE PLASMON
E.G. Bortchagovsky, Yu.V. Demydenko 56

THE KEY ROLE OF THE NiS ELECTRODE/ELECTROLYTE INTERFACE IN LITHIUM ACCUMULATORS
R. Apostolova, E. Shembel, B. Markovsky, D. Aurbach 57

ELECTRICAL PROPERTIES OF $As_2 S_3 Ge_8$ - Te THIN FILMS GROWN FROM THE VAPOR PHASE
Marina Ciobanu, Dumitru Tsiulyanu 58

GAS FILLED PHOTONIC CRYSTAL RESONATORS: PROPERTIES AND APPLICATION IN SENSING AND METROLOGY
E.Ya Glushko 59

OPTICAL CHARACTERIZATION OF HYBRID PEDOT:PSS/SI HETEROSTRUCTURES BY SPECTROSCOPIC ELLIPSOMETRY
O.S. Kondratenko, S.V. Mamykin, T.S. Lunko, I.B. Mamontova, V.R. Romanyuk 60

ELECTRICAL PROPERTIES OF THIN FILMS CdTe DOPED Ca AND Li
Tetiana Mazur, Bogdan Dzundza, Volodymyr Prokopiv 61

INVESTIGATION OF NANOPARTICLES SOLUTIONS BY OPTICAL METHODS
N.A.Davidenko, I.I.Davidenko, N.G.Chuprina, V.V.Kravchenko, E.V. Mokrinskaya, V.A.Pavlov, S.L.Studzinsky 62

CdTe FILMS AS A MATERIAL FOR SOLAR CELLS: STUDYING THE ELECTRICAL CHARACTERISTICS
Semikina T.V., Mamykin S.V., Shmyryeva L.N. 63

ADVANCED SPIN-VALVE TYPE NANOSTRUCTURES WITH WEAKLY FERROMAGNETIC AND ANTIFERROMAGNETIC SPACERS
A.I. Tovstolytkin, A.F. Kravets, D.M. Polishchuk, Ya.M. Lytvynenko, V.Yu. Borynskyi and V. Korenivski 64

EFFECT OF LOW MOLECULAR WEIGHT ARENES ADDITIVES ON THE INTERPHASE LAYER STRUCTURE OF SAN-PS SYSTEMS AND DIELECTRIC BEHAVIOR OF SUCH COMPOSITIONS
Anoshenko M., Bazylyuk T., Iukhymenko N., Budzinska V. 65

GROWTH, CRYSTAL STRUCTURE AND OPTICAL PROPERTIES OF Al-DOPED ZnO THIN FILMS
A. Kashuba, H. Ilchuk, R. Petrus, B. Andriyevsky, O. Bovgyra, I. Semkiv, M. Kovalenko, V. Dzikovskyi 66

ELECTRICAL PROPERTIES OF ZnO THIN FILMS DEPOSITED BY RF-MAGNETRON SPUTTERING
Semikina T.V., Vasin A.V., Rusavsky A.V., Mamykin S.V., Nazarov A.N. 67

THIN SOLID FILMS OF PHOSPHORYLATED CALIX[4]ARENES: STRUCTURE AND SENSORY PROPERTIES
Z.I. Kazantseva , I.A.Koshets, V.I.Kalchenko[b] 68

NANOSTRUCTURED CuI THIN FILMS ON BIODEGRADABLE 69

NANOCELLULOSE FLEXIBLE SUBSTRATES FOR UV-SHIELDING APPLICATIONS
N.P. Klochko, V.A. Barbash, K.S. Klepikova, V.R. Kopach, O.V. Yashchenko, D.O. Zhadan, S.I. Petrushenko, S.V. Dukarov, V.M. Sukhov, A.L. Khrypunova

CARBON SCREEN PRINTED ELECTRODES MODIFIED WITH COMPOSITE FILMS BASED ON SILICA FOR H_2O_2 DETERMINATION 70
Anastasiia Kornii, Anna Borets, Vladyslav V. Lisnyak, Oksana Tananaiko

ULTRA-THIN SILICON TEXTURING FOR FLEXIBLE PHOTOVOLTAICS 71
Viktoriia Koval, Mykhailo Dusheyko, Valerii Barbash

STRUCTURE OF DIAMONDOID THIOL MONOLAYERS ON GOLD: AN STM STUDY 72
Ya.Yu. Lopatina, T.S. Zhuk, A.A. Fokin, A.A. Marchenko

SUPERHYDROPHOBIC TEXTILES WITH FIBERS COATED BY NANOSCTRUCTURED INDIUM-DOPED ZINC OXIDE LAYERS 73
N.P. Klochko, I.V. Khrypunova, K.S. Klepikova, V.R. Kopach, D.O. Zhadan, S.I. Petrushenko, S.V. Dukarov, V.M. Lyubov, M.V. Kirichenko

DESIGN AND CHARACTERIZATION OF FUSED IMINOPYRIDINE POLYMER-BASED FLUORESCENT PROBES 74
Makeiev A.M., Milokhov D.S., Keda T.Ie., Khilya O.V., Volovenko Yu.M.

DETERMINATION OF Pb(II) CONCENTRATION IN AQUEOUS MEDIUM ON NANOCRYSTALLINE TiO_2/Y THIN-FILM ELECTRODE 75
I. Medyk, V. Vorobets, G. Kolbasov, A. Garashchenko, S. Oblovatna, S. Karpenko, N. Antonyuk

PECULIARITIES OF $CuInSe_2$ LAYERS FABRICATION 76
V. Nicorici, P. Chetrus

THE INFLUENCE OF THE LIGAND NATURE ON THE ELECTROCHEMICAL PARAMETERS OF THE TIN FILMS AS ANODE MATERIALS FOR LITHIUM ION BATTERIES 77
V.S. Kublanovsky, N.I. Globa, V.M. Nikitenko, E.A. Babenkov, Yu.V. Shmatok

GROWTH, CRYSTAL STRUCTURE AND OPTICAL PROPERTIES OF $CdTe_{1-x}Se_x$ THIN FILMS PREPARED BY QUASI CLOSE-SPACE SUBLIMATION METHOD 78
R. Petrus, H. Ilchuk, A. Kashuba, I. Semkiv, N. Ukrainets

STUDY OF THE FORMATION OF GLASS ENAMEL COATINGS PART FOR STEEL PIPES 79
An. Salei, V. Goleus, T. Kozyreva

USING Ti-CONTAINING STAINLESS STEEL AND ALUMINIUM FOIL COMPOSITES FOR BENZENE VAPOR PHOTODESTRUCTION 80
Sanzhak O.V., Brazhnyk D.V., Goncharov V.V., Zazhigalov V.A.

THERMAL STABILITY AND VISCO-ELASTIC PROPERTIES OF THE FILMS ON THE BASIS OF EPOXY-OLIGOESTERIC MIXTURES 81
Olena Shyshchak, Olena Astakhova, Michael Bratychak

ELECTRO- AND PHOTOELECTROPHYSICAL PROPERTIES OF NEW PHOTOSENSITIVE THIN FILM STRUCTURES BASED ON ANIONIC σ-COMPLEXES 82
Studzinsky S.L., Siniugina A.T.

SYNTHESIS OF LANTHANUM COBALTITE FROM ACETYLACETONATE COMPLEXES LaCo(AA)$_5$·nD 83

L.I. Sliusarchuk, L.I. Zheleznova, T.V. Pavlenko, O.O. Rogovtsov, O.K. Trunova
PHOTOELECTROCHEMICAL PROPERTIES OF COPPER VANADATE 84
V.O. Smilyk, S.S. Fomanyuk, G.Ya. Kolbasov, I.A. Rusetskii
PHOTOELECTRET PROPERTIES OF PHOTOSENSITIVE POLYMERIC COMPOSITES DOPED BY TRIARYLMETHANE DYES 85
Studzinsky S.L.
EFFECT OF NANOSTRUCTURING TO RESPONSE KINETICS OF TELLURIUM THIN FILMS BY NITROGEN DIOXIDE SENSING 86
Dumitru Tsiulyanu, Marina Ciobanu, Olga Mocreac
PHOTOTHERMOPLASTIC RECORDING MEDIA AND ITS APPLICATION IN THE HOLOGRAPHIC METHOD OF DETERMINATION OF REFRACTIVE INDEX OF LIQUID AND GASEOUS OBJECTS 87
Studzinsky S.L., Pavlov V.A., Chuprina N.G., Kuranda N.N., Mokrinskaya E.V., Kravchenko V.V., Davidenko N.A, Davidenko I.I.
CRITICAL CURRENT IN HIGH-Tc SUPERCONDUCTOR BICRYSTALS WITH LOW-ANGLE [001]-TILT GRAIN BOUNDARIES 88
A.L. Kasatkin, V.P. Tsvitkovskyi
CATALYTIC PROPERTIES OF CoRe AND CoWRe ALLOYS IN THE HYDROGEN ELECTROREDUCTION REACTION 89
T. Maltseva, Yu. Yapontseva, V. Kublanovsky
THIN-FILM STRUCTURES BASED ON Ge - GeO_2 - B_2O_3 AND Ge - ZnS (ZnO) - B_2O_3 SYSTEMS FOR INTERFERENCE OPTICS OF IR SPECTRUM RANGE 90
V. Zinchenko, I. Magunov, O. Mozkova, G. Volchak
THE PRECONCENTRATION OF AROMATIC ALDEHYDES ON POLYDIMETHYLSILOXANE-DIVINYLBENZENE FIBER 91
A.O. Mosendz, V.M. Levchyk, M.F. Zui

SECTION 4. Electronic processes in nanostructures and polymer composites

FEATURES OF RAMAN SCATTERING AND X- RAY DIFFRACTION IN As-Se-Te(S) CHALCOGENIDE GLASSES DOPED BY SAMARIUM 93
R.I. Alekberov, A.I. Isayev, S.I. Mekhtiyeva
INFLUENCE OF GAMMA RADIATION ON THE ELECTRICAL PROPERTIES OF EXTRUDED SAMPLES OF SOLID SOLUTION $Bi_{85}Sb_{15}$ <Te> 94
Abdullayeva I.A., Abdinova G.D., Tagiyev M.M.
EXCITONIC EFFECTS IN AGGREGATES OF ORGANIC DYES AND CARBONIC NANOSTRUCTURES 95
Alexander P. Demchenko
THE NATURE OF OVERTONES AND COMBINATIONS OF FUNDAMENTAL VIBRATIONAL MODES IN RAMAN SCATTERING SPECTRA OF LEAD PHTHALOCYANINE FILMS 96
M.P.Gorishnyi, O.M.Fesenko
PECULIARITY OF INELASTIC CHARACTERISTICS OF NANOCOMPOSITES MULTIWALLED CARBON NANOTUBES AND POLYETHYLENE, POLYVINYL CHLORIDE, POROUS POLYSTYRENE, RADIATION CROSS-LINKED HYDROGELS 97
A.P. Onanko, M.P. Kulish, Y.A. Onanko, N.V. Kutsevol, O.N. Nadtoka, D.V. Charnyi, O.P. Dmytrenko, T.M. Pinchuk-Rugal, M.A. Aleksandrov, O.L. Pavlenko, T.O. Busko, P.P. Ilyin, O.M. Rozhkovskiy

MANIFESTATION OF THE SPECIAL NANO-STRUCTURAL PROPERTIES OF LAYERED TRANSITION METAL DIHALCOGENIDES AND GRAPHENE WITH CHANGE IN THE NUMBER OF MONO-LAYERS
Kornienko N.E., Naumenko A.P., Gubanov V.O. 98

SPECTROSCOPIC STUDY OF ELECTRONIC INTERACTIONS IN “NANOCRYSTAL-MOLECULE” SYSTEMS
V. Dzhagan, O. Selyshchev, O. Isaeva, N. Mazur, O. Raievska, O. Stroyuk, D.R.T. Zahn 99

PECULIARITY OF IONEXCHANGE, ABSORBING PROPERTIES OF NANOCOMPOSITES MULTIWALLED CARBON NANOTUBES AND POLYETHYLENE, POLYVINYL CHLORIDE, POROUS POLYSTYRENE, SiO_2
A.P. Onanko, M.P. Kulish, Y.A. Onanko, D.V. Charnyi, O.P. Dmytrenko, T.M. Pinchuk-Rugal, M.A. Aleksandrov, O.L. Pavlenko, T.O. Busko, P.P. Ilyin, L.I. Kurochka 100

RESONANCE LASER INDUCTION OF THE ELECTRON DENSITY WAVES AND OBSERVATION OF ACOUSTIC MODES IN THE RAMAN SPECTRA OF NANO AND MICROCRYSTALLITES OF MoS_2
Kornienko N.E., Naumenko A.P. 101

METABOLIC ELECTRON TRANSFER BY FRAGMENTS OF DNA MOLECULE TAKING INTO ACCOUNT THE REAL STRUCTURE OF NUCLEOTIDES
A. D. Suprun, L. V. Shmeleva 102

SYNTHESIS, MORPHOLOGY AND INTRAMOLECULAR STRUCTURE OF POLYETHYLENE GLYCOL WITH METHYLENE BLUE DYE FILMS
M.A. Alieksandrov, T.M. Pinchuk-Rugal, A.M. Gaponov, O.P. Dmytrenko, A.P. Onanko, M.P. Kulish 103

SYNTHESIS AND PROPERTIES OF NANOSTRUCTURED COMPOSITE $Ce:GdAG/Cr:Al_2O_3$
I.V. Berezovskaya, O.V. Khomenko, N.I. Poletaev, M.E. Khlebnikova, V.P. Dotsenko 104

SOLVENT EFFECTS ON PHOTOPHYSICAL PROPERTIES OF ORGANIC DYES IN THE POLYMER MATRIX
T.V. Bezrodna, O.I. Antonenko, L.F. Kosyanchuk, O.O. Brovko, V.I. Bezrodnyi, A.M. Negriyko 105

ABSORPTION OF LASER RADIATION BY METALLIC NANOPARTICLES EMBEDED IN A DIELECTRIC MATRIX IN THE CONDITIONS OF SURFACE PLASMON RESONANCE
A.A. Biliuk, O.Yu. Semchuk, O.O. Havryliuk 106

pH-SENSITIVE PHOTOLUMINESCENCE OF $AgInS_2/ZnS$ QUANTUM DOTS IN BUFFER SOLUTIONS
L. Borkovska, A. Rachkov, J.-L. Doualan 107

MICROELLIPSOMETRIC INVESTIGATIONS OF MIM STRUCTURES WITH ORDERED LATTICES OF PLASMONIC NANOPARTICLES
E. Bortchagovsky, F. Dai, J. Tang, M. Fleischer, I. Milekhin, D. Zahn, R. Kenaz, R. Rapaport 108

EXCITONS SPECTRUM IN MULTILAYER AlN/GaN NANOSTRUCTURES
Igor Boyko, Halyna Tsupryk, Yuriy Stoianov 109

$Pb_{1-X}Cd_XI_2$ LAYERED SEMICONDUCTOR NANOSCINTILLATOR FILMS: 110

OPTICAL AND STRUCTURAL PROPERIES
A.P. Bukivskii, Yu.P. Gnatenko, P.M. Bukivskii, I.V. Fesych
EFFECT OF NITROGEN DOPING ON THE REDOX PROCESSES ON THE SURFACE OF GRAPHEN-CLUSTERS 111
Demianenko E.M., Grebenyuk A.G., Lobanov V.V., Karpenko O.S., Kartel N.T
SURFACE CENTERS OF Cr^{3+} IONS IN NANOSIZED Al_2O_3
V.P. Dotsenko, I.V. Berezovskaya, N.I. Poletaev, M.E. Khlebnikova, O.V. Khomenko, N.P. Efryushina 112
POSITRON SPECTROSCOPY STUDY OF DEFECTS STRUCTURE AND ELECTRONIC PROPERTIES OF POLYMER-CARBON NANOTUBE COMPOSITES 113
E. Tsapko, E. Len, I. Galstian, M. Rud
PHOTOELECTROPHYSICAL PROPERTIES OF PHOTOSENSITIVE THIN FILM STRUCTURES BASED ON HETEROLIGAND TETRAAMINE CHROMIUM(III) COMPLEXES 114
Gerda V.I., Studzinsky S.L.
DONOR-ACCEPTOR INTERMOLECULAR ELECTRON BONDING AND STRUCTURAL TRANSFORMATIONS OF CHAIN-LIKE BISMUTH PENTAFLUORIDE CLUSTERS 115
Grebenyuk A.G.
DISPERSION OF VIBRATIONAL AND ELECTRONIC STATES AND FINE SPIN-DEPENDENT STRUCTURE OF THEIR ENERGY LEVELS IN HEXAGONAL BN CRYSTALS 116
V. Gubanov, A. Naumenko, I. Dotsenko
SPECTRAL PROPERTIES OF NILE RED DYE AT THE SILICA NANOSURFACE AND LIQUID MEDIA 117
Khristenko I. V., Vasilieva A. V., Ivanov V. V.
ELECTRONIC AND MAGNETIC PROPERTIES OF NITROGEN/IRON-DOPED GRAPHENE-LIKE HEXAGONAL NANOCLUSTERS 118
Karpenko O.S., Demianenko E.M., Lobanov V.V., Kartel M.T.
OPTICAL ABSORPTION OF POLYAMINOARENES DOPED WITH ELECTRON ACCEPTOR NANOCLUSTERS 119
Konopelnyk O.I., Rabiy V.I., Aksimentyeva O.I.
DYNAMICS OF ELECTRON TRANSFER IN MELANIN-TRINITROFLUORENONE SYSTEM 120
A.O. Kostetskyi, Yu.P.Piryatinski, A.B.Verbitsky[1], P.M.Lutsyk[2], A.Rozhin

POLYMER-POLYMER COMPOSITES BASED ON WATER-SOLUBLE POLYMERS AND POLYANILYLINE 121
V. Dutka, Ya. Kovalskyi, O. Aksimentyeva, T. Virsta, H. Halechko
IONIC CONDUCTIVITY OF GLYCOPOLYMER NETWORKS BASED ON XANTHAN AND BLOCKED POLYISOCYANATE IN THE PRESENCE OF GLICEROL 122
Nataly Kozak, Katerina Didenko, Zoja Gagolkina, Stanislav Nesin
SPECTROSCOPIC INVESTIGATION OF CHLORINE-BASED PHOTOSENSITIZERS IN POLYMER MATRIX 123
A. Naumenko, N. Kutsevol, V. Zorin

CORRELATION BETWEEN STRUCTURAL AND SPECTROSCOPIC PROPERTIES OF Sm^{3+}-DOPED $MgAl_2O_4$ NANOCRYSTALLINE SPINEL
K. Lamonova, I. Danilenko, O. Gorban, G. Volkova, S. Orel, Yu. Pashkevich, O. Viagin, P. Maksimchuk, V. Seminko, Yu. Malyukin, V. Kurnosov 124

INFLUENCE OF POLYMER MORPHOLOGY AND METHOD OF COMPOSITE SYNTHESIS ON THE DIELECTRIC PROPERTIES OF NANOCARBON COMPOSITES
Lazarenko O., Syvolozhskyi O., Zhuravkov O., Matzui L. 125

PHOTOLUMINESCENCE IN GAS ENVIRONMENTS ZnO NANOPOWDERS DOPED BY In AND Ga
I.V. Lazoryk, Yu.I. Venhryn, A.S. Serednytski, D.I. Popovych 126

EFFECT OF ELECTRON SCATTERING BY IMPURITY ON THE ELECTRONIC STRUCTURE, TYPE AND SPATIAL CHARACTERISTICS OF NANOSCALE REGIONS OF MAGNETIC ORDERING IN ALLOYS
E. G. Len, V. V. Lizunov, T. D. Shatnii, M. V. Ushakov, T. S. Len 127

THE INFLUENCE OF GATE POTENTIAL ON THE FORMATION OF ELECTROLUMINESCENCE IN A MOLECULAR PHOTODIODE
V.O. Leonov, Ye.V. Shevchenko, E.G. Petrov 128

STRUCTURAL AND OPTICAL STUDY OF GLUTATHIONE-CAPPED Ag–In–S NANOCRYSTALS
B.V. Lopushanska, Y.M. Azhniuk, D. Solonenko, V.V. Lopushansky, I.P. Studenyak, D.R.T. Zahn 129

COMPLEX PERMITTIVITY OF EPOXY COMPOSITES WITH CARBON NANOTUBES AND TiO_2 IN MICROWAVE RANGE
O.V. Lozitsky, L.L. Vovchenko, L.Y. Matzui, V.V. Zagorodnii, V.V. Oliynyk 130

STUDY OF EXCITED STATE RELAXATION IN SUBSTITUTED POLYENES BY TIME-RESOLVED ELECTRON SPECTROSCOPY (TRES)
K. O. Maiko, D. O. Merzhyievskyi, O. V. Shablykin, Yu. P. Piryatinski, I. M. Dmytruk, Ya. O. Prostota, N. V. Obernikhina, O .D. Kachkovsky, V. S. Brovarets 131

ELECTRICAL AND THERMAL PROPERTIES OF EPOXY COMPOSITES FILLED WITH CARBON NANOTUBES AND INORGANIC PARTICLES
Len T.A., Vovchenko L.L., Turkov O.V., Lozitsky O.V., Matzui L.Yu. 132

LOW ENERGY ELECTRON INDUCED PLASMON EXCITATIONS IN THE W (100)
M. O. Vasylyev, I. M. Makeeva, V. M. Kolesnik, V. I. Patoka 133

SURFACE PROPERTIES OF METAL FILLED COMPOSITE BASED ON POLYMER BLEND
Misiura A., Mamunya Ye., Prochazka M., Omastova M., Kulish M., Pylypenko A. 134

CARBON NANOTUBES AS MODIFIERS OF PROPERTIES OF MATERIALS
H.Yu. Mykhailova 135

FORMATION OF DONOR-ACCEPTOR COMPLEXES IN FULLERENE SOLUTIONS
Nagorna T.V., Bulavin L.A., Chudoba D. 136

PECULIARITIES OF THE SPECTRAL PROPERTIES OF BORON-CONTAINING DYES IN THE AQ3 MATRIX
O.M. Navozenko, V.M. Yashchuk, M.Yu. Losytskyy, A.P. Naumenko, I.Yu. Doroshenko, Yu.L. Slominskii, D. Gudeika 137

FIELD-CONTROLLED ELECTRON TRANSPORT IN CHOLESTERIC LIQUID CRYSTAL – CARBON NANOTUBES COMPOSITE 138
Yu.I. Olenych, Yu.Yu. Horbenko, O.I. Aksimentyeva, I.B. Olenych, I.D. Karbovnyk

THE INFLUENCE OF PHOSPHORUS AND CHLORINE AS ACTIVE LAYERS FOR ELECTRONIC GAS SENSORS 139
A. Pud, N. Ogurtsov, O. Kukla, Yu. Noskov, J.-L. Wojkiewicz, V. Bliznyuk, A. Mamykin, I. Myronyuk

FEATURES OF CYANINE AGGREGATES FORMATION IN NANOPOROUS MATRICES 140
I. Ropakova, A. Sorokin, I. Bespalova, S. Yefimova, Yu. Malyukin

ESTIMATION OF DIPOLE MOMENTS FOR THE PHENALENONE DYES IN LIQUID AND POLYMER POLAR MEDIA 141
T.V. Bezrodna, L.F. Kosyanchuk, O.M. Roshchin, V.I. Bezrodnyi, G.V. Klishevich, V.I. Melnyk

THE STUDY OF TiO_2/SnO_2 COMPOSITION AFTER IT SONOCHEMICAL AND MECHANOCHEMICAL TREATMENT 142
Sachuk O.V., Zazhigalov V.A., Diyuk O.A., Tsyba M.M.

SILVER NANOPARTICLES EFFECT ON THE SENSITIZATION OF DYE-SENSITIZED SOLAR CELLS 143
Temirbayeva D.A., Seliverstova E.V., Ibrayev N.Kh., Ishchenko A.A.

ANALYSIS OF THE PROPERTIES OF METALLOORGANIC COMPOUNDS WITH THE Fe^{3+} NANOPROBES BY EPR METHOD 144
Shapovalov V.A., Aksimentyeva E.I., Shavrov V.G., Koledov V.V., Shapovalov V. V., Tkach V.I.

EFFECT OF NON-METAL ADMIXTURES ON THE ELECTRONIC STRUCTURE AND XPS CHARACTERISTICS OF TITANIA NANOPARTICLES 145
O.V. Smirnova, A.G. Grebenyuk, V.V. Lobanov

CONTROL OF THE EXCITON SELF-TRAPPING IN LUMINESCENT MOLECULAR AGGREGATES 146
A. Sorokin, I. Grankina, S. Yefimova, Yu. Malyukin

TWO STAGE INTERCALATION OF MULTYWALL CARBON NANOTUBES WITH COBALT 147
D. O. Spylka, I. V. Ovsiienko, T. A. Len, L. Yu. Matzui, F. Le Normand, T. L. Tsaregradskaya, G. V. Saenko[a]

ELECTRIC PROPERTIES OF NI-C AND CO-C CORE-SHELL NANOPARTICLES IN POLYMER MATRIX 148
O. A. Syvolozhskyi , O. S. Yakovenko, L. Yu. Matzui, L. L. Vovchenko, V.V. Vilchinskyi, V.M. Bogatyrov

MAGNETOTHERMOELECTRIC PROPERTIES OF BULK NANOSTRUCTURED SAMPLES OF $Bi_{85}Sb_{15}$ SOLID SOLUTION 149
Tagiyev M.M.

ELECTRON TRANSPORT IN GRAPHENE: COMBINED EFFECTS OF STRAINS AND DEFECTS 150
Valentyn A. Tatarenko, Taras M. Radchenko

THE TUNING OF ACID-BASE AND PROTON CONDUCTIVITY PROPERTIES OF THE TITANIA NANOSTRUCTURES BY CAREFULLY DOPING 151
G. Telbiz, N.Vlasenko, E.Leonenko, P. Smertenko, T Kavetskyy, P.Strizhak,

IMPACT OF FILM MORPHOLOGY ON ELECTRONIC STRUCTURE IN THE PROTOTYPICAL SEMICONDUCTING POLYMER POLY-3-HEXYLTHIOPHENE 152
A. Vakhnin, A. Kadashchuk, A. Zhugayevych, A. Kohler

SORPTION-LUMINESCENCE METHOD FOR DETERMINATION OF YTTERBIUM AND MORIN USING TRANSCARPATHIAN CLINOPTILOLITE 153
O. Stashkiv, V. Vasylechko, R. Gamernyk, G. Gryshchouk, A. Zelinskiy

ENHANCEMENT OF RADIOLUMINESCENCE IN CERIUM DOPED MIXED OXYORTHOSILICATE NANOCRYSTALS $Lu_{2-x}Y_xSiO_5:Ce^{3+}$ 154
V. Seminko, P. Maksimchuk, I. Bespalova, O. Viagin, A. Aslanov, Yu. Malyukin

INFLUENCE OF SILVER NANOPARTICLES ON PHOTOELECTROCHEMICAL CHARACTERISTICS of TiO_2-GO NANOCOMPOSITE 155
Sadykova A.E., Zhumabekov A.Zh., Ibrayev N.Kh.

ELECTRIC PROPERTIES OF GaSe <$NaNO_2$+PROPOLIS> NANOHYBRID ENCAPSULATE 156
Maksymych V., Ivashchyshyn F., Chabecki P.

PLASMONIC NANOCAVITY METASURFACE BASED ON LASER-STRUCTURED SILVER SURFACE AND SILVER NANOPRISMS FOR THE ENHANCEMENT OF ADENOSINE NUCLEOTIDE PHOTOLUMINESCENCE 157
A. V. Tomchuk, O. A. Yeshchenko, V. Yu. Kudrya, I. M. Dmitruk, N. I. Berezovska, P. O. Teselko, S. Golovynskyi, B. Xue, J. Qu

SECTION 5. Nonlinear properties of polymer composites, nanostructures, NLO information recording

INFLUENCE OF ELECTROTHERMOPOLARIZATION ON PE+$PbCrO_4$ –BASED NANOCOMPOSITION STRUCTURES 159
M.A. Ramazanov, A.S. Huseynova, F.V. Hajiyeva, S.U. Atayeva

HIGH QUALITY PATTERNS PRODUCED BY NONLINEAR LASER LITHOGRAPHY FOR LIQUID CRYSTAL ALIGNMENT 160
I. Pavlov, A. Rybak, A. Dobrovolskiy, Z. Kazantseva, A. Bek, O. Candemir, R. Kravchuk, I. Gvozdovskyy

SYNTHESIS OF NOVEL POLYAZOMETHINE WITH ANTIPYRINE MOIETY: EFFECT OF COPOLYMER COMPOSITION VARIATION ON NONLINEAR OPTICAL RESPONSE 161
V. Ovdenko, V. Multian, D.Komarenko, O. Kolendo, V. Gayvoronsky

A DUAL-WAVELENGTH PULSED LASER PROCESSING PLATFORM FOR A-SI THIN FILM CRYSTALLIZATION 162
V. Türker, M. E. Yağcı, S. H. Salman, K. Çınar, S. K. Eken, A. Bek

INFLUENCE OF SUBSTITUENTS ON PHOTORESPONSIVE BEHAVIOR OF METHACRYLIC POLYMERS CONTAINING 8-HYDROXY-QUINOLINE AZO-DYES IN SIDE-CHAIN 164
D. Chomicki, O. Kharchenko, A. Kozanecka-Szmigiel, D. Szmigiel, Ł. Skowroński, J. Kowalonek, V. Smokal, O. Krupka, B. Derkowska-Zielinska

SURFACE-INDUCED PHOTOREFRACTIVE EFFECT IN LIQUID CRYSTAL CELLS CONTAINING GOLD NANOPARTICLES 165
A. Gridyakina, H. Bordyuh, S. Bugaychuk, L. Viduta, V. Styopkin

NONLINEAR PROPERTIES OF MAGNETO-OPTIC DYNAMICS OF FERRONEMATIC LIQUID CRYSTALS 166
Korostil A.M., Krupa M.M.

PLASMON SPECTRA AND OPTICAL CUBIC NONLINEARITY OF THREE-LAYER SRUCTURES: Au NANOPARTICLES - Al_2O_3 - PdO (Pd) 167
Brodin O.M., Brodyn M.S., Liakvovetskyi V.R., Rudenko V.I., Styopkin V.I

SYNTHESIS AND NONLINEAR OPTICAL CHARACTERIZATION OF NOVEL AZO- AND AZOMETHINE CONTAINING POLYMERS WITH HETEROCYCLIC MOIETY 168
V.M. Ovdenko, V. V. Multian, A. V. Uklein, I. V. Kulai, O.Yu. Kolendo, V. Ya. Gayvoronsky

NONLINEAR LASER PROCESSING IN OPTICAL MATERIALS 169
S. Pavlova, V. Kadan, E. Yagci, K. Eken, I. Pavlov

DIBENZOFLUORENE DERIVATIVE FOR NONLINEAR OPTICS AND SOLAR CELLS APPLICATIONS 170
A. El Haimeur, I. V. Levkov, T. V. Yegorova, A. I. Kysil, H. Bakkali, E. Blanco, Z. V. Voitenko

ANALYSIS OF THE FORMATION OF RELAXATION ZONES ON A SOLID SURFACE BY LASER NANOSTRUCTURING OF A MATERIAL 171
O.V. Yushchenko[a], O.S. Krivets

SECTION 6. Novel materials, structures, and technologies

POLYDOPAMINE AS AN EFFICIENT SORBENT FOR URANIUM EXTRACTION FROM NATURAL ENVIRONMENTS 173
V.N. Bliznyuk, K. Kołacińska, A.A. Pud, N.A. Ogurtsov, Y.V. Noskov, B.A. Powell, T.A.DeVol

NON-DESTRUCTIVE DEPTH PROFILE RECONSTRUCTION OF INTERFACE BETWEEN BIOMOLECULES AND CARBON-BASED SURFACE USING ANGLE-RESOLVED XPS 174
A. Artemenko, O. Babčenko, E. Ukraintsev, M. Marton, M. Vojs, T.Wårgberg, A. Kromka

2,7-DIMETHOXYCARBAZOLE AND TRIAZINE BASED BIPOLAR MATERIALS FOR OLEDs: SYNTHESIS AND INVESTIGATION 175
A. Bucinskas, A. Gruodyte, O. Bezvikonnyi, D. Volyniuk, J. V. Grazulevicius

STIMULATED EMISSION OF MEROCYANINE DYE IN POROUS ALUMINIUM OXIDE MATRIX 176
D.A. Afanasyev, N.Kh. Ibrayev, A.A. Ishchenko

IR-FOURIER TRANSFORM SPECTROSCOPIC STUDY OF SYSTEMS NaNO-Al_2O_3 + NaNO-SiO_2 + H_2O 177
Agayev T.N., Melikova S.Z., Tagiyev M.M., Dzhafarova S.Z.,Akhmedova A.M.

NOVEL HYBRID TITANIUM-CONTAINING INTERPENETRATING POLYMER NETWORKS WITH EFFICIENT UV-INDUCED CHARGES SEPARATION 178
Tetiana T. Alekseeva , Nataly V. Kozak, Nataly V. Iarova

ELECTRON AND HEAT TRANSPORT IN SnTe CRYSTALS WITH VARIOUS VACANCY CONCENTRATIONS IN TIN LATTICE 179
T.D. Aliyeva, G.Z. Bagiyeva, N.M. Akhundova*, G.D. Abdinova, B.Sh. Barkhalov

THE MECHANISM OF EPOXY COMPOUND AND ADIPIC ACID REACTION 180
Olena Astakhova, Olena Shyshchak, Michael Bratychak

THERMODYNAMIC FUNCTIONS OF PHASE TRANSITIONS OF COMPOUNDS A_8GeX_6 (A=Ag, Cu; X=S, Se) 181
Bayramova U.R., Mashadiyeva L.F., Shukurova G.M.,Babanly M.B.

ACRYLIC ACID MODIFIED LDH FOR NANOSTRUCTURED POLYMER MATERIALS 182
I. Bei, V. Budzinska, O. Slisenko, O. Tolstov, N. Iukhymenko

PULSED IR LASER CRYSTALLIZATION OF AMORPHOUS SILICON FILMS 183
Kamil Çınar, Alpan Bek

SYNERGISTIC EFFECTS DURING THE OBTAINING OF POLYVINYLPYRROLIDONE NICKEL-FILLED COPOLYMERS 184
B. Berezhnyy, O. Grytsenko, O. Suberlyak, N. Baran, A. Fechan

PROPERTIES OF MICROWAVE CURED EPOXY-ANHYDRIDE COMPOUNDS 185
O. Bilogubka

NEW STRUCTURE HOST MATERIALS FOR PHOSPHORESCENT OLED DEVICES 186
Do. Blazevicius, D. Tavgeniene, M. Eidimtas, G. Krucaite, B. Zhang, S. Sutkuviene and S. Grigalevicius

DESIGN OF PLASTIC SCINTILLATORS FOR DETECTION OF VARIOUS TYPES OF RADIATION 187
V.N. Bliznyuk, A.F.Seliman, N.A.Derevyanko, A.A.Ishchenko, S.M.Husson, T.A.DeVol

LUMINESCENT INVESTIGATIONS OF CADMIUM SULFIDE NANOWHISKERS 188
A. Bogoslovska, D. Grynko, E. Bortchagovsky

CRYSTALLINE SILICON WAFER SLICING BY DEEP SUBSURFACE LASER INDUCED MODIFICATION FOLLOWED BY SELECTIVE CHEMICAL ETCHING 189
M. Zolfaghari Borra, H. Nasser, B. Radfar, I. Pavlov, R. Turan, A. Bek

PHENOL-BASED OLIGOMERS WITH REACTIVE FUNCTIONAL GROUPS 191
Michael Bratychak

DEFINING THE CONDITIONS FOR THE FORMATION OF OXIDE FILMS DURING THE ELECTROCHEMICAL OXYDATION OF THE Ti_6Al_4V ALLOY IN ETHYLENEGLYCOL SOLUTIONS 192
O. Bukhinik, S. Gura, A. Pilipenko

SYNTHESIS AND PROPERTYS OF ARYLFLUORENYL SUBSTITUTED DERIVATIVES OF BRIDGED-TRIPHENYLAMINE AND TRIPHENYLAMINE FOR OPTOELECTRONIC APPLICATIONS 193
M. Cekaviciute, J. Simokaitiene, J.V. Grazulevicius, D. Volyniuk, G. Sini

THERMODYNAMIC OF METHYLENE BLUE ADSORPTION ON THE HYBRID TiO_2 / DIATOMITE NANOCOMPOSITE 194
Datsko T., Zelentsov V.

BURST MODE ULTRAFAST LASER WITH NOVEL PULSE STRECHING FOR MICROMACHINING 195
M. E.Yağcı, V. Türker, S. Pavlova, E. Tunçkol, S. K. Eken, I. Pavlov

DEVELOPMENT OF ANTIMICROBIAL MATERIALS BASED ON PLA/MEDITERRANEAN PROPOLIS AND THYMUS VULGARIS ESSENTIAL OIL 196
Hocine Djidjelli, Nacera Chibani, Nadjet Ardjoum

OPTIMISATION OF LASER-INDUCED SURFACE STRUCTURES FOR SENSITIVITY OF THEIR SPECTRAL CHARACTERISTICS TO CHANGES IN THE ENVIRONMENT 197

I. Dmitruk, N. Berezovska, O. Yeshchenko, O. Stanovyi, E. Hrabovsky, P. Teselko, A. Dmytruk, I. Blonskyi
SOME PHYSICO-CHEMICAL ASPECTS OF THE PREPARATORY STAGES OF THE FORMATION OF SELF-CLEANING PHOTOCATALYTICALLY ACTIVE COATINGS 198
O. Dryuchko, D. Storozhenko, N. Bunyakina, I. Ivanytska, I. Gornitsky, K. Kytaihora, V. Khaniukov
PICOSECOND LASER PROCESSING OF STAINLESS STEEL FOR SUPERHYDROPHOBIC SURFACE FABRICATING. 199
Dupliak Ivan, Yuchen Liang, Guozhu Yan, Fenping Li, Ivaniuk Khystyna
Ni-Co/SiO$_2$ COMPOSITES: SURFACE STRUCTURE AND MORPHOLOGY 200
Dyachenko A., Ischenko O., Goncharuk O., Borysenko M.
PbI$_2$:Cd^{2+} NANOCLUSTERS SYNTHESIZED BY ONE-STEP DEPOSITION METHOD 201
O.G. Dziazko, I.V. Fesych, O.O. Bondar, S.A. Nedilko, T.A. Voitenko, M.A. Zelenko, V.V. Lendel, A.P. Bukivskii, P.M. Bukivskii, O.V. Ivanov
RED MUD AS A CATALYST FOR THE DECOMPOSITION OF SODIUM BOROHYDRIDE 202
Fedchenko Anastasiia, Brychenko Iryna, Ivanenko Iryna, Kosogina Iryna
THE PROCESS OF NICKEL NANOPARTICLE FORMATION IN HYDROPHILIC POLYMER / INORGANIC MATRICES 203
T.B. Zheltonozhskaya, N.M. Permyakova, A.S. Fomenko, D.O. Klymchuk, V.V. Klepko, L.N. Grishchenko, L.O. Vretik
COMPOSITIONAL EFFECT ON THERMOTROPIC PHASE TRANSITIONS IN LONG-CHAIN *n*-ALKANOIC ACIDS BINARY MIXTURES 204
T.A. Gavrilko, I.I. Gnatyuk, V.I. Styopkin, N.D. Shcherban, J. Baran, M. Drozd
DISTRIBUTION INHOMOGENEITY OF NEMATIC 5CB CONFINED TO MOLECULAR SIEVES BY FTIR SPECTROSCOPY AND CARS IMAGING 205
I. Gnatyuk, A. Dementjev, T. Gavrilko, R. Karpicz, J. Baran, N. Shcherban
ORGANIC BIPOLAR EMITTERS FOR OLEDs AND OXYGEN SENSORS 206
J. V. Grazulevicius, N. Kukhta, R. Pashazadeh, E. Skuodis, A. Tomkeviciene, R. Keruckiene, J. Simokaitiene, M. Cekaviciute, X. Tan, D. Volyniuk, K. Ivaniuk, P. Stakhira
SYNTHESIS AND PROPERTIES OF D-A-D-TYPE ORGANIC SEMICONDUCTING MATERIALS BASED ON A FLUORENONE MOIETY 207
D. Gudeika, O. Bezvikonnyi, D. Volyniuk, J. V. Grazulevicius
THERMAL HYSTERESIS IN SPIN-CROSSOVER NANOCRYSTALS WITH (ANTI)FERROMAGNETIC SURFACE 208
Iu. Gudyma, A. Maksymov
REFINEMENT OF THE PHASE DIAGRAM OF THE Bi-Se SYSTEM AND THERMODYNAMIC PROPERTIES OF THE BISMUTH SELENIDES 209
Zeynalova G.S., Mammadova A.T., Aghazade A.I., Imamaliyeva S.Z., Babanly M.B.
CALCIUM CARBONATE IN THE FORM OF SPHERICAL PARTICLES: SYNTHESIS AND PROPERTIES 210
N.V. Guzenko, O.L. Gabchak, O.I. Oranska
SYNTHESIS AND CHARACTERIZATION OF PHOTOSENSITIVE CHIRAL DOPANT FOR APPLICATIONS IN LIQUID CRYSTALS 211

V. O. Chornous, M. V. Vovk, Yu. V. Dmytriv, A. V. Rudnichenko, M. V. Skorobahatko, L. N. Lisetski, I. A. Gvozdovskyy

UTILIZATION OF A NEW DESIGNED ELECTROMECHANICAL REACTOR FOR HEAVY METALS REMOVAL IN AN INDUSTRIAL WASTEWATER TREATMENT PROCESS USING ORGANIC AND INORGANIC MATERIALS 212
Amir Hajiali

UNDERSTANDING THE ORIGIN OF THE CHANGE OF THE ENANTIOSELECTIVITY IN THE CYCLOADDITION STEP IN THE THE REACTION MECHANISM OF ENANTIOSELECTIVE REDUCTION OF KETONES WITH BORANE CATALYZED BY A *B*-METHOXY OXAZABOROLIDINE CATALYST DERIVED FROM (–)-B-PINENE: A DFT STUDY 213
Hichem Sadrik Kettouche

SURFACE MORPHOLOGY OF NANOSTRUCTURED GAS SENSORS BASED ON METAL-POLYMER COMPOUNDS 215
D.O. Harbuz, A.P. Pospelov, M.D. Romanov, P.V. Mateychenko, A.P. Konotop, V.A. Gudimenko, G.V. Kamarchuk

COBALT-IRON SPINEL / REDUCED GRAPHENE OXIDE COMPOSITE MATERIAL FOR SUPERCAPACITOR APPLICATIONS 216
M. Hodlevska, R. Zapukhlyak, V. Boychuk, V. Kotsyubynsky, K. Bandura, A. Kachmar, M. Hodlevskyi

DIELECTRIC AND MAGNETIC PROPERTIES OF $KTaO_3$:Li,Co CERAMICS 217
S. V. Lemishko, O. O. Andriiko, M. M. Prokopiv, M. Trepachko, I. S. Golovina

NEW RECORDING MEDIA FOR HOLOGRAPHY BASED ON AZO-DYES OF SUDAN SERIES 218
Valeriia Ovdenko, Dmitry Vyshnevsky, Nikolay Davidenko, Valeriy Pavlov

NEW PHASES OF VARIABLE COMPOSITION BASED ON FAMATINITE MINERAL - POTENTIAL ENVIRONMENTAL FRIENDLY THERMOELECTRIC MATERIALS 219
Ismailova E.N., Mashadiyeva L.F., Shevelkov A.V, Bakhtiyarly I.B., Babanly M.B.

HIGH-ε CERAMICS FOR EPR RESONATOR INSERT 220
S. V. Lemishko, V. O. Yukhymchuk, I. P. Vorona, I. S. Golovina, S. O. Solopan, A. G. Belous

EFFECT OF ORTHO- AND PARA-SUBSTITUTIONS IN AZO-NAPHTHOL DYES ON THE DIFFRACTION EFFICIENCY OF HOLOGRAPHIC MEDIA 221
D. Vyshnevsky, V. Ovdenko, A. Ishchenko, I. Kurdyukova, N. Davidenko, E. Mokrinska, V. Pavlov

INNOVATIVE SENSOR SOLUTIONS BASED ON YANSON POINT CONTACTS 222
G.V. Kamarchuk, A.P. Pospelov, A.V. Yeremenko, L.V. Kamarchuk, A.V. Kravchenko

CHEMICAL TREATMENT OF Cd (Mn)Te SURFACE 223
L.M. Kanak, V.G. Ivanitska, P.M. Fochuk

OPTICAL PROPERTIES OF THE NEW 10-((1,3,4-OXADIAZOLES-2-YL)METHYL)ACRIDINE-9(10H)-ONES 224
Yu. V. Karpenko, A. I. Panasenko

FEATURES OF TRANSFORMATIONS IN SYSTEMS OF NITRATE PRECURSORS OF LANTHANOIDS AND ALKALINE METALS IN THE 225

FORMATION OF PHOTOCATALYTIC ACTIVE NANO-LAYERED PEROVSKITE-LIKE PHASES
O. Dryuchko, D. Storozhenko, N. Bunyakina, I. Ivanytska, I. Gornitsky, V. Khaniukov, K. Kytaihora

INFLUENCE OF SUBSTITUENT ON POLYMERIZATION ABILITY OF METHACRYLIC MONOMERS BASED ON AURONE FRAGMENT 226
O. Kharchenko, D. Shyrchenko, V. Smokal, O. Krupka

PECULIARITIES OF ELECTRON-PHONON INTERACTION IN THE INDIUM SELENIDES:*Ab INITIO* INVESTIGATION 227
L.Yu.Kharkhalis, K.E.Glukhov, T.Ya.Babuka, M.V.Liakh

THE PRODUCTS OF SO_2 INTERACTION WITH ALCOHOL SOLUTIONS OF TRIS(HYDROXYMETHYL)AMINOMETHANE 228
Khoma R.E., Dlubovskiy R.M., Baumer V.N., Ennan A.A.-A., Ishkov Yu.V., Vodzinskiy S.V., Gelmboldt V.O.

SYNTHESIS, CRYSTAL, AND MOLECULAR STRUCTURES OF 3d-METAL 5-SULFOSALICYLATE-BENZOHYDRAZIDE COMPLEXES 229
Koksharova T.V., Savchenko O., Mandzii T.V.

NEW 2-OXOIMIDAZOLIDINE DERIVATIVES: DESIGN, SYNTHESIS AND EVALUATION OF ANTI-BK VIRUS ACTIVITIES IN VITRO 230
Kornii Yurii, Oleh Shablykin, Volodymyr Brovarets

POLYMER COATED MAGNETIC NANOPARTICLES 231
Korobeinyk A.V., Tertykh V.A.

EVALUATION OF THE POLYURETHANE BASED LASER ELEMENTS PHOTOSTABILITY AND BEAM STRENGTH 232
L. Kosyanchuk, N. Kozak, N. Babkina, T. Bezrodna,V. Bezrodnyi, O. Antonenko

PREPARATION OF POLYLACTIC ACID/SILICA COMPOSITES USING THE *IN SITU* RING-OPENING POLYMERIZATION OF LACTIDE 233
Kozakevych R.B., Polyshchuk L.M., Tertykh V.A.

ACTIVATED CARBON (AC) – TITANIUM DIOXIDE (TiO_2) COMPOSITES: EFFECT OF AC PROPERTIES ON PHOTOCATALYTIC EFFICIENCY 234
Anzhela Kukh, Irina Ivanenko, Igor Astrelin

SYNTHESIS AND CHARACTERIZATION OF CdS NANOPARTICLES GROWN IN THE STAR-LIKE COPOLYMER 235
Yu. Kuziv, H. Hrytsko, N. Melnik, V. Pavlenko, N. Kutsevol

PHYSICO-CHEMICAL BASES FOR THE PREPARATION OF POLYMER-INORGANIC (NANO)COMPOSITES 236
G. Dudok, I. Dziaman, N. Semenyuk, K. Kysil, V. Skorokhoda

STUDIES OF THE PHYSICAL, OPERATIONAL AND OPTICAL-SPECTRAL CHARACTERISTICS OF THE HIGHLY TRANSPARENT TOLUENESULFONAMIDE AND BENZGUANAMINEFORMALDEHYDE POLYMERS 237
Vladimir Lebedev, Tetiana Tykhomyrova

MAGNETOTHERMAL PROPERTIES OF LANTHANUM MANGANITE PEROVSKITE NANOPARTICLES 238
C. Song, N.A. Liedienov, A.V. Pashchenko, I.V. Fesych, V.G. Pogrebnyak, G.G. Levchenko

LUMINESCENT PROPERTIES OF Cd(II) COORDINATION POLYMER 239

ASSEMBLED FROM 2-THIOPHENECARBOXYLIC ACID AND 1,2-BIS(PYRIDIN-4-YLMETHYLENE)HYDRAZINE LIGANDS
V. N. Lozovan, O. V. Kulikova, V. Ch. Kravtsov, E. B. Coropceanu, M. S. Fonari

SPR DETECTION OF URANIUM IN AQUEOUS MEDIA USING POLYDOPAMINE FILMS 240
S. Mamykin, I. Gnilitskyi, M. Dusheyko, T. DeVol, V. Bliznyuk

COMPLEXES OF COBALT AND NICKEL FUMARATES WITH BENZOHYDRAZIDE AND PHENYLACETIC ACID HYDRAZIDE. SYNTHESIS, CRYSTAL, AND MOLECULAR STRUCTURES 241
Mandzii T.V., Savchenko O., Koksharova T.V.

EFFECT OF ADDITION OF THE MONOMERS BASED ON 4′-METHACRYLOXYAURONES ON THERMAL STABILIZATION OF POLYSTHYRENE. 242
A. Martynes-Harsiia, N. Iukhymenko, A. Kolendo

DESIGN, SYNTHESIS AND INVESTIGATION OF 1,8-NAPHTHALIMIDE BASED COMPOUNDS 243
N. Masimukku, D. Gudeika, D. Volyniuk, J. V. Grazulevicius

NANOSIZED Pt-SnO_2 GAS SENSITIVE MATERIALS FOR CREATION SEMICONDUCTOR SENSORS TO HYDROGEN 244
Matushko I.P., Oleksenko L.P., Maksymovych N.P., Lutsenko L.V., Fedorenko G.V.

RESEARCH OF MORPHOLOGY OF WORKING SURFACES OF CONTACTS AND PHYSICAL MECHANICAL PROPERTIES OF ECOLOGICALLY SAFE ELECTRIC CONTACT MATERIALS 245
Korobsky V.V., Mrachkovsky A.M.,

RESEARCH OF THE PHASE COMPOSITION OF AUTOCLAVE AND NON-AUTOCLAVE AERATED CONCRETE CONTAINING FERROSILICON AS A GASIFIER 246
A.O. Musina, O.O. Sihunov, T.V. Kravchenko, A.O. Hura

INFLUENCE OF THE METHOD OF OBTAINING GAS SENSITIVE MATERIALS ON CHARACTERISTICS OF CO-CONTAINING SENSORS CREATED ON THEIR BASE 247
Matushko I.P., Maksymovych N.P., Oleksenko L.P., Scolyar G.I., Ripko O.P.

BENZOPHENONE PHENOTHIAZINE-5,5-DIOXIDE MATERIAL EXHIBITING PHOTO-INDUCED CONFORMATIONAL REARRANGEMENTS 248
E. Narbutaitis, M.Guzauskas, D. Volyniuk, J. V. Grazulevicius

THIN NANOPOROUS GRAPHITIC FILMS FABRICATED BY MAGNETRON PLASMA CHEMICAL VAPORE DEPOSITION FROM ACETYLENE 249
A.Nazarov, O.Slobodian, A.Rusavsky, Yu.V.Gomeniuk, N.Pavlusiak, A.Vasin, T.Nazarova, O.Gudymenko, O.Khyzhun, V.Stepanov, D.Kisyl

MOLECULAR RELAXATIONS IN MODIFIED MICROCRYSTALLINE CELLULOSE 250
Alekseev O., Lazarenko M., Nedilko S.G., Revo S., Scherbatskii V., Teselko P., Prokopets V.. Hamamda S., Dorbani T., Naoui Y., Boyko V., Sheludko V., Gomenyuk O.

FLUORESCENCE PROPERTIES INTERACTION INTERFERON A2B WITH OLIGO- AND MONORIBONUCLEOTIDES 251
R.O. Nikolaiev, Ye.Yu. Stepanenko, S.I. Chernykh, Z. Yu. Tkachuk

NEW PARAMAGNETIC CENTER IN Cu-DOPED Y-STABILIZED ZrO_2 252
V.V. Nosenko, I.P. Vorona, S.M. Okulov, L.Yu. Khomenkova, N.O. Korsunska

SYNTHESIS AND CHARACTERIZATION OF A NEW $Sn_{1-x}Mn_xBi_2Te_4$ SOLID SOLUTIONS AS A POTENTIAL MAGNETİC TOPOLOGICAL INSULATORS 253
E.N. Orujlu, Z.S. Aliev, M.B. Babanly

EXCITATION DYNAMIC IN NEW TYPE DETECTORS BASED ON STILBENE 254
R. Karpicz, L.Valkunas, N. Ostapenko, Yu. Ostapenko , O.Kerita, N. Galunov, I. Lazarev, Ya. Polupan

HYBRID-CONTROLLED SYNTHESIS OF COBALT NANOPARTICLES IN AQUEOUS SOLUTIONS 255
N.M. Permyakova, T.B. Zheltonozhskaya, D.O. Klymchuk, V.V. Klepko, L.N. Grishchenko, A.S. Fomenko, L.O. Vretik

NEW CARBAZOLE-π-BRIDGE-TRIAZOLE COMPOUNDS FOR OLED APPLICATIONS 256
N. Pokhodylo, R. Lytvyn, M. Stanicka, M. Tupychak, Kh. Pitkovych, O. Bezvikonnyi, E. Urbonas, D. Volyniuk, S. Kutsiy, K. Ivaniuk, V. Kinzhybalo, P. Stakhira, A. Tomkeviciene, J.V. Gražulevičius, M. Obushak

NEW CONDUCTING POLYMER NANOSTRUCTURED COMPOSITES FOR ECOLOGICAL MONITORING AND PROTECTION 257
A. Pud, N. Ogurtsov, M. Petrychuk, V. Oliynyk, V. Zagorodnii, O. Kruglyak

A NEW OPERATING PRINCIPLE OF SELECTIVE DETECTION IN GASES 258
A.V. Savytskyi, G.V. Kamarchuk, A.P. Pospelov, A.O. Herus, Yu.S. Doronin, V.L. Vakula, E. Faulques

THE EFFECT OF BUTIL ALCOHOL ON ANODIC BRASS OXIDATION PROCESSES IN PHOSPHATE ELECTROLYTES 259
Silchenko D., Shkolnikova T., Pancheva H., Pilipenko A.

EFFECTS OF CHARGE ORDERING IN ELECTRONIC SUBSYSTEM OF QUASI-2D BEDT-TTF CONDUCTORS 260
Yu. Skorenkyy, O. Kramar, Yu. Dovhopyatyy

SYNTHESIS AND PHOTOLUMINESCENCE OF SILICA AND SILICA-TITANIA HYBRID MATERIALS DOPED WITH LANTHANIDE EDTA- AND DTPA-CHELATES 261
S.S. Smola, E.M. Fadieiev, N.V. Rusakova, I.V. Berezovskaya

SILVER DOPED TIO_2-LDH CLAY NANOCOMPOSITES FOR PHOTOCATALYTIC REDUCTION OF CARBON DIOXIDE 262
Starukh H., Petryk I., Koci K.

INVESTIGATION OF MONTMORILLONITE INTERCALATION BY POLYVINYLPYRROLIDONE AND OBTAINING TERMOPLASTIC NANOCOMPOSITES 263
O. Suberlyak, V. Krasinskyi, O. Nikitchuk

SOME FEATURES OF EFFECTIVE STACKING INTERACTIONS IN AROMATIC POLYAMIDES 264
A.V. Tokar, O.P. Chigvintseva

NANOCOMPOSITE POLYMER SENSOR MATERIALS FOR DETECTION OF HEAVY METAL ION CONTAMINANTS IN WASTE WATER 265
O. Zinchenko, V. Ezhova, O. Slisenko, A. Tolstov

THE BACTERICIDAL MATERIAL POLYURETHANE FOAM-I_2 BASED ON THE 266

SORPTION OF IODINE FROM AQUEOUS AND ORGANIC SOLUTIONS
A. Yu. Trokhimenko
STRUCTURE AND MORPHOLOGY OF CRYPTOMELANE SAMPLES SYNTHESIZED BY DIFFERENT METHODS AND THEIR ACTIVITY IN THE REACTION OF SULFUR DIOXIDE OXIDATION WITH AIR OXYGEN 267
T.L. Rakitskaya, A.S. Truba, A.P. Nazar, T.A. Kiose, V.Y. Volkova
SOLIDPHASE EQUILIBRIA IN THE GeTe-Bi$_2$Te$_3$ SYSTEM AND CRYSTAL STRUCTURES OF THE INTERMEDIATE PHASES 268
Alakbarova T.M, Orijlu E.N., Imamaliyeva S.Z., Babanly M.B.
TEMPERATURE-TRIGGERED AGGREGATION OF PNIPAM-BASED CORE/SHELL NANOPARTICLES 269
L.O. Vretik, O.M. Chepurna, A.I. Marynin, O.A. Nikolaeva, T.Y. Ohulchanskyy
KINETICS OF FREE RADICAL POLYMERIZATION OF METHYL METHACRYLATE INITIATED BY PENTAZADIENES 270
Vyshnevsky D., Syromiatnikov V., Kolendo A.
ORGANO-MINERAL COMPOSITE POLY(4 –VINYLPYRIDINE–*b*-STYRENE)-SILICA GEL: SYNTHESIS AND SORPTION PROPERTIES 271
M. Tovstenko-Zabelin, E.S. Yanovska, O. Kondratenko, O.A. Nikolaeva, D. Sternik, I.O. Savchenko, L.O. Vretik
COMPOSITION AND MOLECULAR WEIGHT DISTRIBUTION OF SUBSTANCES FROM NATURAL COFFEE EXTRACTS 272
Kurta S. A., Khatsevich O.M., Yakubiak M.R.
ADSORPTION PROPERTIES OF NATURAL ALUMOSILICATE UKRAINIAN MINERALS, *IN SITU* MODIFIED BY POLY [8-METHACROYLOXYQUINOLINE] TO Pb(II), Mn(II), Cu(II) AND Fe(III) IONS 273
I. Savchenko, E. Yanovska, D. Sternik, O. Kychkyruk
FLUORESCENT TECHNIQUES FOR REGISTRATION OF DRUG REDISTRIBUTION FROM NANOSIZED CARRIERS 274
V. Zorin, T. Zorina, I. Kravchenko, N. Kutsevol

SECTION 7. Nanocomposites and lasers in medicine and biology

MORPHOLOGICAL AND PROPERTIES CHARACTERIZATION OF NOVEL BIOCOMPOSITES OF POLY(3-HYDROXYBUTYRATE-CO-3-HYDROXYHEXANOATE) (PHBHHx)/ALOE VERA FIBERS 276
Mustapha Kaci, Nadjet Dehouche, Celia Idres, Idris Zembouai, Stéphane Bruzaud
AGGREGATIVE STABILITY OF RARE-EARTH BASED NANOPARTICLES IN DIFFERENT MICROENVIRONMENTS AND BIOLOGICAL MEDIA 277
Katherine Averchenko, Nataliya Kavok, Ganna Grygorova, Vladimir Klochkov
EFFECT OF DIFFERENT DOSES OF SILVER NANOPARTICLES IN POLYMER MATRIX TREATMENT ON FEMALE REPRODUCTIVE FUNCTION IN MICE 278
Sribna V., Kaleinikova O., Kuziv Y., Lytvynenko A., Vinogradova-Anyk O., Karvatskiy I., Voznesenskaya T., Blashkiv O., Kutsevol N.
ECO-FRIENDLY SYNTHESIS OF Ag$_2$S NANOPARTICLES, THEIR OPTICAL AND ANTIMICROBIAL PROPERTIES 279
M. Borova, A. Naumenko, O. Kapush, S. Plokhovska, I. Horiunova, A. Yemets
INTERPLAY OF ANTIBIOTIC GRAMICIDIN S WITH CHOLESTEROL AND DEXTRAN-POLYACRYLAMIDE COPOLYMERS IN LIPID MEMBRANES 280
L.V. Budianska, V.P. Berest, N.V. Kutsevol, Y.I. Kuziv, O.V. Vashchenko

CHEMICALLY CROSS-LINKED HYBRID HYDROGELS FOR PROLONGED RELEASE OF ANTIBIOTICS 281
Oksana Nadtoka, Volodymyr Doroschuk, Serhii Lelyushok, Nataliya Kutsevol
APPLICATION OF INTERNAL CAPACITANCE COMPENSATION OF REACTIVE POWER IN SINGLE-PHASE INDUCTION MOTORS 282
Zablodskiy M.M., Chuenko R.M.
THERMAL ASSISTED ANTI-STOKES LUMINESCENCE AND LASER COOLING EFFECT OF TRICARBOCYANINE DYES 283
O.P. Dimitriev, O.M. Fedoryak, I.P. Sharanov, Yu.L. Slominskii
HOST–GUEST COMPLEXES OF MEFENAMIC ACID AND β-CYCLODEXTRIN DERIVATIVES: SPECTROSCOPIC STUDY 284
G.V. Grygorova, V.K. Klochkov, S.L. Yefimova, Yu.V. Malyukin
CONTROLLED PRO/ANTIOXIDANT ACTIVITY OF $GdYVO_4:Eu^{3+}$ NANOPARTICLES 285
K.O. Hubenko, S.L. Yefimova, P.O. Maksimchuk, N.S. Kavok, V.K. Klochkov, Yu.V. Malyukin
PHOTDYNAMIC THERAPY IN THE TREATMENT OF PATIENTS WITH NEUROPATHIC AND ISCHEMIC DIABETIC FOOT SYNDROME 286
Tetiana Kharchenko, Oksana Melekhovets, Yuriy Melekhovets, Alevtuna Radko
IN SILICO APPROACHES IN DRUG DESIGN OF NOVEL ANTIOXIDANT AGENTS 287
Olena Klenina, Volodymyr Ogurtsov, Borys Zimenkovsky
STRUCTURAL CHARACTERIZATION, ELECTROMAGNETIC AND THERMODYNAMIC PROPETRIES OF POULTRY BY-PRODUCTS 288
M. M. Zablodskij, S. I. Kovalchuk
INTERPHASIC INTERACTIONS IN MIXTURES OF HYDROPHOBIC AND HYDROPHILIC SILICA 289
V.V. Turov, T.V. Krupskaya, M.T. Kartel
USE OF PHOTODYNAMIC THERAPY FOR TREATMENT OF CHRONIC ULCERS 290
B. V. Krysa, V. M. Krysa
IN VITRO RESEARCH ON DEGRADATION OF 60S BIO-CERAMIC IMPLANT MATERIALS 291
Kusyak A.P., Chornyi V.S., Dubok V.A.
NANOCOMPOSITES FOR ANTICANCER THERAPY 292
Nataliya Kutsevol, Yuliia Kuziv, Vasyl Chekhun, Vladimir Zorin, Michel Rawiso
ENHANCEMENT OF THE X-RAY PDT NANOSYSTEM EFFICIENCY BY THE PRESENCE OF HfO_2 NANOPARTICLES 293
Losytskyy M.Y., Vretik L.O., Nikolaeva O.A., Degoda V.Y., Shcherbakov O.B., Podust G.P., Doroshenko I.P., Ohulchanskyy T.Y., Yashchuk V.M.
EVALUATION OF ACID-BASE SURFACE PROPERTIES OF NANOSCALE Fe_3O_4 BY POTENTIOMETRIC TITRATION 294
Kusyak N.V., Kusyak A.P., Petranovska A.L., Gorbyk P.P.
GREEN SYNTHESIS AND ADSORPTION PROPERTIES OF COBALT FERRITES 295
M. Liaskovska, T. Tatarchuk
BINDING OF Zr PHTHALOCYANINES WITH BETA-LACTOGLOBULIN: SPECTRAL-FLUORESCENT STUDY 296

Losytskyy M.Y., Chernii S.V., Chornenka N.V., Tretyakova I.M., Chernii V.Y., Kovalska V.B.
LIGHT-INDEPENDENT PRO-OXIDANT ACTIVITY OF UV PRE-IRRADIATED ORTHOVANADATE NANOCRYSTALS 297
P. Maksimchuk, V. Omielaieva, K. Hubenko, V. Seminko, S. Yefimova, Y. Malyukin
HYBRID HYDROGELS LOADED WITH BIOLOGICAL ACTIVE DYES AS MATERIALS FOR THERAPEUTIC DELIVERY 298
Nadtoka Oksana, Virych Pavlo, Kutsevol Natalia, Martynyuk Victor
CHRONIC VENOUS DISEASE CEAP 1-2 TREATMENT WITH 1064 Nd:YAG LASER 299
V. Mishura, Y. Melekhovets, V.l Pak, O.Melekhovets, O. Sytnik
RESEARCH OF WORK OF A ROOFTOP SOLAR POWER PLANT IN HOT WATER SUPPLY SYSTEMS OF STUDENT DORMITORIES 300
Nalyvaiko V., Radko I., Okushko O., Mrachkovska N. Antypov Ie.
SYNTHESIS OF POLYMERIC HYDROGELS INCORPORATING CHLORHEXIDINE AS ANTIBACTERIAL WOUND DRESSINGS 301
Oksana Nadtoka, Pavlo Virych, Vasyl Krysa, Nataliya Kutsevol
NANOPARTICULAR AGENTS FOR NEAR INFRARED LUMINESCENCE BIOIMAGING AND IMAGING GUIDED THERAPY 302
T.Y. Ohulchanskyy
PHOTOINACTIVATION OF *STAPHYLOCOCCUS AUREUS* WITH MONOCHROMATIC LOW ENERGY VISIBLE LIGHT 303
Pavlo Virych, Oksana Nadtoka, Petro Virych, Victor Martynyuk, Nataliya Kutsevol
FORMATION AND DYNAMICS OF OXYGEN VACANCIES IN CeO_2-ZrO_2 AND CeO_2-Y_2O_3 NANOCRYSTALS 304
Okrushko O., Seminko V., Maksimchuk P., Malyukin Yu.
MASS SPECTROMETRY STUDY OF NANOBIOCOMPLEXES FORMATION BETWEEN DIMETHYL SULFOXID AND ANTIMICROBIAL AGENTS 305
V. Pashynska, M. Kosevich, A. Gomory
PHOTODYNAMIC THERAPY AS A NEW APPROACH IN THE ACNE VULGARIS TREATMENT 306
Radko A.S., Melekhovets O.K., Kharchenko T.O., Melekhovets Yu.V.
PONDEROMOTIVE FORCES AS A REASON FOR DESTRUCTION OF VIRUS INTERACTING WITH NANOPARTICLES 307
V. Lozovski, N. Rusinchuk, V. Lysenko, M. Lokshyn, S. Zagorodnya, M. Chayka, Yu. Mukha, N. Vityuk
ELABORATION OF NEW APPROACHES FOR PREPARATION OF HIGHLY SENSITIVE CONDUCTOMETRIC BIOSENSORS FOR L-ARGININE DETERMINATION 308
O.Y. Saiapina, S.V. Dzyadevych
IMPROVING ANTIOXIDANT PROPERTIES OF NANOCERIA BY DOPING AND LASER IRRADIATION 309
V. Seminko, P. Maksimchuk, G. Grygorova, E. Okrushko, Y. Malyukin
FILM HYDROGELS WITH SILVER NANOPARTICLES FOR THE TREATMENT OF BURNS AND WOUNDS 310
V. Skorokhoda, N. Semenyuk, Y. Melnyk, M. Bratychak, G. Dudok
IMPROVEMENT OF THE METHOD FOR DETERMINING ENERGY 311

CONSUMPTION IN A BIOGAS REACTOR
M.M. Zablodskiy, M.O. Spodoba,

MULTIFUNCTIONAL $ReVO_4$:Eu^{3+} NANOPARTICLES IN THERANOSTICS
S.L. Yefimova, P.O. Maksimchuk, K.O. Hubenko, V.K. Klochkov, Yu.V. Malyukin 312

DETERMINATION OF OPTIMUM APEX ANGLE OF CONE-SHAPED PART OF PELLETIZER DIE BY MEANS OF SIMULATING BIOMASS GRANULATION PROCESS
Polishchuk Viktor, Tarasenko Svitlana, Antypov Ievgen, Bilyk Stepaniia 313

SECTION 8. Physics and technology of organic solar cells, LEDs, FETs, sensors, conjugated thin films for electrochromic devices.

SYNTHESIS AND CHARACTERIZATION OF ELECTROACTIVE MATERIALS FOR AIEE PROPERTIES
R. S.e Bernard, G. Sych, S. Nasiri, O. Bezvikonnyi, D. Volyniuk, A. Ariffin, V. Andrulevicienė, J. V. Grazulevicius 315

ELECTROOPTICAL TRANSITIONS IN CONJUGATED POLYMER SYSTEMS
Aksimentyeva O.I. 316

DERIVATIVES OF TRIAZINE AND *TERT*-BUTYLCARBAZOLE AS TADF EMITTERS FOR OLEDS
O. Bezvikonnyi, D. Gudeika, D. Volyniuk, J. V. Grazulevicius 317

THE INFLUENCE OF MgO ADDITION ON RED PHOTOLUMINESCENCE OF Mn^{4+} ACTIVATED Zn_2TiO_4 PHOSPHORS
L. Borkovska, T. Stara, I. Vorona, V.Nosenko, K.Kozoriz, C. Labbé, J. Cardin, J.-L. Doualan 318

ORGANIC-INORGANIC NANOSTRUCTURED SENSING MATERIALS WITH TUNABLE ADSORPTION PROPERTIES
J. Burlachenko, I. Kruglenko, B.Snopok 319

STRUCTURE, OPTICAL AND SENSORY PROPERTIES OF POLY-3,4-ETHYLENEDIOXYTHIOPHENE FILMS DOPED WITH GRAPHENE OXIDE
Horbenko Yu. Yu., Glazunova V. A., Ivaniuk H. B., Matkivska G. M., Vistak M., Starykov G. O., Aksimentyeva O. I. 320

GREEN PHOTOLUMINESCENCE OF N-ANNELATED PERYLENES IN A DISTRIBUTED FEEDBACK CAVITY.
I.Dupliak, A. Bucinskas, Kh. Ivaniuk, H. Petrovska, D. Volyniuk, V. Fitio, P.Stakhira, J. V. Grazulevicius 321

NEW MECHANISM OF THERMAL CONDUCTIVITY OF MOLECULAR SUBSTANCE
A. I. Krivchikov, O. A. Korolyuk, O. O. Romantsova, Yu. V. Horbatenko,
A. Jeżowski, D. Szewczyk 322

NEW STRUCTURE HOLE TRANSPORTING DERIVATIVES FOR PHOSPHORESCENT OLED DEVICES
G. Krucaite, D. K. Dubey, S. S. Swayamprabha, R. A. K. Yadav, D. Blazevicius, J. Tagare, S. Chavhan, T.-C. Hsueh, S. Vaidyanathan, S. Grigalevicius, J.-H.Jou 323

THE INFLUENCE OF PHOSPHORUS AND CHLORINE ORGANIC VOLATILE COMPOUNDS ON THE SENSOR PROPERTIES OF ELECTROCONDUCTIVE COMPOSITE FILMS
Kukla O.L., Mamykin A.V., Pud A.A., Ogurtsov N.A. 324

SOLUTION-PROCESSED WHITE ORGANIC LIGHT-EMITTING DIODE BASED 325

ON TWO EMISSIVE LAYERS
M. Mahmoudi, J. Keruckas, D. Volniuk, J. Simokaitiene, J. V.Grazulevicius
POLYMER ELECTROLYTE MEMBRANES BASED ON PEO-CONTAINING BLOCK COPOLYMERS 326
Larisa Kunitskaya, Tatyana Zheltonozhskaya, Stanislav Nessin, Valeriy Klepko
FEATURES OF THE OPERATION OF BIOSENSORS BASED ON THE PPR EFFECT IN CHROMATIC MODE 327
Kukla O.L., Fedchenko A.N., Vahula O.A., Surovtseva E.R., Shirshov Yu.M.
EFFECT OF POST-PROCESSING ON THE EFFICIENCY OF PEDOT/PSS-Si SOLAR CELLS 328
Mamykin S.V., Lunko T.S., Mamontova I.B., Kondratenko O.S., Kotova N.V.
POLY COMPLEXES BASED UNSATURATED β-DICARBONYLS AND LANTHANIDES FOR ORGANIC LIGHT-EMITTING DIODES 329
Savchenko I.O., Berezhnytska O.S. Ivakha N.B., Trunova E.K.
SYNTHESIS AND STUDIES OF PROPERTIES OF ORGANIC SEMICONDUCTORS CONTAINING DONOR AND ACCEPTOR MOIETIES 330
L. Skhirtladze, J. V. Grazulevicius, A. Bin Ariffin, W. K.Lin
SYNTHESIS AND PROPERTIES OF PHENANTHROIMIDAZOLYL-BASED DERIVATIVES 331
E. Skuodis, R. Zubrevicius, D. Volyniuk, D. Gudeika, J.V. Grazulevicius
IN SITU IMMOBILIZATION ON THE SILICA GEL SURFACE AND ADSORPTION CAPACITY OF POLY [8-METHACROYLOXYQUINOLINE] ON TOXIC METALS IONS 332
I. Savchenko, E. Yanovska, L. Vretik, D. Sternik, O. Kychkyruk
THERMALLY-STIMULATED LUMINESCENCE IN AN OLED HOST MATERIAL DOPED WITH TADF EMITTERS 333
Andrei Stankevich, Alexander Vakhnin, Andrey Kadashchuk
ON THE NATURE OF CURRENT CARRIERS IN INTERPOLYMER COMPLEXES PEDOT:PSS AS COMPONENTS OF SOLAR CELLS 334
O.I. Tkachuk, M.I. Terebinska, Ya.S. Krivoruchko, V.V. Lobanov
COMBINED POLYMER SENSITIVE ELEMENTS FOR GAS SENSORS 335
O. Aksimentyeva, B. Tsizh, Yu. Horbenko, M. Dzeryn
EXCIPLEX-BASED APPROACHES FOR WHITE LIGHT EMITTING DIODES 336
D. Volyniuk, G. Sych, M. Guzauskas, J. Simokaitiene, J. V. Grazulevicius
3-[3-(4-CHLOROPHENYL)-2-(4-FLUOROPHENYL)-2*H*-ISOINDOL-1-YL]-1-PHENYLPYRROLIDINE-2,5-DIONE AS A CANDIDATE FOR SOLAR CELLS APPLICATIONS 337
A. El Haimeur, I. V. Levkov, T. V. Yegorova, A. I. Kysil, H. Bakkali, E. Blanco, Z. V. Voitenko
NEW MATERIALS BASED ON COMPLEXES AND METALOPOLYMERS OF EUROPIUM (III) 338
Berezhnytska O.S., Rohovtsov O.O., Fedorov Ya. V., Savchenko I.O., Trunova O.K.
PROPERTIES OF POLYHEXAFLUORPROPYLENE THIN FILMS 339
K. Grytsenko, Yu. Kolomzarov, P. Lytvyn, V. Ksianzou, S. Schrader
Biologically active compounds based on silver complexants 340
Myhalchuk A.O., Sikors'ka K.A, Kamenska T.A., Berezhnytska O.S.
SELF-ASSEMBLED DICHROIC ORGANIC SOLIDS 341

K. Grytsenko, P. Lytvyn, Y. Kolomzarov, Y. Slominskii, V. Kurdiukov, O. Navozenko
SYNERGETIC EFFECT STUDY IN TWO-COMPONENT MIXTURES OF ASCORBIC ACID WITH AMINO ACIDS 342
Hocharenko A., Chygyrynents O
LASER TEXTURING OF SILICON SOLAR CELLS AS AN ALTERNATIVE TO CHEMICAL WET ETCHING 343
O. Candemir, E. Genc, H. Ciftpinar, H. Nasser, M. Zolfaghari Borra, A. Bek, R. Turana, and I. Pavlov
PHOTOCONDUCTIVITY IN POLYETHYLENE-SEMICONDUCTOR (p-GaSe) COMPOSITE 344
Babayeva R.F., Abdinov A.Sh., Amirova S.I.
PHOTOELECTRET EFFECT IN POLYMER-PHOTOSENSITIVE SEMICONDUCTOR n-InSe COMPOSITES 345
Dzhafarova S.Z., Babaeva R.F., Ragimova N.A., Abdinov A.Sh.
AUTHOR INDEX 346
CONTENTS 360

Наукове видання

12th International Conference «Electronic Processes in Organic and Inorganic Materials» (ICEPOM-12)

(КАМ’ЯНЕЦЬ-ПОДІЛЬСЬКИЙ, 1–5 ЧЕРВНЯ 2020)

МАТЕРІАЛИ ТЕЗ ДОПОВІДЕЙ ТА ВИСТУПІВ

(АНГЛІЙСЬКОЮ МОВОЮ)

Комп’ютерна верстка В. Овденко, Д. Вишневський