



# **ABSTRACT BOOK**

**Summer school**

**International research  
and practice conference:**

**NANOTECHNOLOGY  
AND NANOMATERIALS  
(NANO-2017)**

**19 - 26 August 2017  
Migove-Chernivtsi region  
Ukraine**



Group photo of participants of the 1st International Summer School for young scientists "NANOTECHNOLOGY: from fundamental research to innovations" (Bukovel 2012)



Interview with Prof. Dr. Thomas A. Klar, Director of the Institute of Applied Physics, Johannes Kepler University of Linz, Austria



At the lecture during the 1<sup>st</sup> International Summer School



Summer school participants on the background of the monument, which is a symbol of the geographical center of Europe (Rakhiv district)



Closing ceremony of the 1<sup>st</sup> International Summer School for young scientists "NANOTECHNOLOGY: from fundamental research to innovations"



Group photo of the 2<sup>nd</sup> International Summer School participants  
(Bukovel 2013)



Summer School participant PhD.  
Vorokhta M. (Czech Republic)  
tries to play trembita



Plenary Session



The organizing committee  
working hard



PhD. Lyashchova A.G.  
(Ukraine)



Group photo of 3<sup>rd</sup> International Summer School participants  
(Yaremche 2014)



Discussion with speaker



Hiking the path of Dovbush,  
Carpathians



Director of Institute of Physics of  
NAS of Ukraine Prof.  
Leonid Yatsenko awards prizes to  
the winners of competition



Interview with Prof. Leonid  
Chernozatonskiy from Prokhorov  
Institute of general physics (Russia)



## Venue

Previous Schools was held in Bukovel, Yaremche and Lviv. You can find some information about this venues.



Bukovel is located on the territory of the Carpathian National park not far from the highest point of the Carpatian Mountains. Mountains around Bukovel connected with a picturesque meadow, opening a wonderful view to the primeval nature of the Carpathians and charming mountain landscapes.



Yaremche is situated in the picturesque Prut River valley, this little town is one of the most famous tourist centers of the Carpathian region.



Formerly capital of the historical region of Galicia, Lviv is now regarded as one of the main cultural centres of today's Ukraine.

**THE 4-th INTERNATIONAL  
SUMMER SCHOOL  
NANOTECHNOLOGY:  
FROM FUNDAMENTAL RESEARCH  
TO INNOVATIONS**

**19-26 AUGUST 2017,  
MIGOVE-CHERNIVTSI REGION,  
UKRAINE**

**BOOK OF ABSTRACTS**

УДК 536:669

**The International Summer School “Nanotechnology: from fundamental research to innovations”.** Book of abstracts of young scientists and lecturers of the International Summer School, 19–26 August, 2017. Edited by Dr. Olena Fesenko. – Lviv: Eurosvit, 2017. – P. 108.

ISBN 978-966-8364-93-1

This book consists of abstracts of young Scientists from Europe, Ukraine and other countries who received grants for participation in International Summer School “Nanotechnology: from fundamental research to innovations” that was held in Migove, Ukraine from 19–26 August, 2017. This International Summer School gave the opportunity to young researchers and early-career scientists to participate in a series of lectures on the emerging fields of Nanosciences & Nanotechnologies. Top class experts from universities and research institutions from different countries of the World shared their knowledge and experience in the format of lecture presentations and round table discussions. Summaries of lectures are also included in this book.

International Summer School was held by the Institute of Physics of NAS of Ukraine and partners: Yuriy Fedkovych Chernivtsi National University (Ukraine) and Representative office of Polish Academy of Sciences in Kyiv (Poland).

The abstracts and lectures cover such currently important topics as microscopy of nanostructures, nanocomposites, nanostructured interfaces and surfaces, nanooptics, nanoplasmonics and enhanced vibrational spectroscopy.

Web-site of Summer School:

[http://www.iop.kiev.ua/~summer\\_school](http://www.iop.kiev.ua/~summer_school)

ISBN 978-966-8364-93-1

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2017

**Welcome to the International Summer School  
on Nanotechnology for Young Scientists!**



Nanotechnology is becoming an important field of diagnostics in physics, chemistry and medicine. You should be proud to contribute to this field.

I remember that I was kind of anxious, when I had to present my first talk on a conference with important professors. But you know your results better than them. Make them curious to learn about your results. If you present a poster, look also at the other posters and discuss with the poster presenters. Ask “stupid” questions! You may learn a lot in this way. Make scientific friends!

Last not least enjoy science!

**Dr. Andreas Otto**



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**4-th INTERNATIONAL SUMMER SCHOOL**

**NANOTECHNOLOGY:**

**FROM FUNDAMENTAL RESEARCH  
TO INNOVATIONS**

## **Session 1**

### **Nanochemistry and Biotechnology**

## **Investigation of catalase activity adsorbed on the gold nanoparticles surface**

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The use of proteins and enzymes for therapeutic purposes requires the maintenance of sufficient activity during in vivo treatment. Many proteins exhibit short half-life in vivo and therefore require carrier structures to selectively transport them to diseased cells or tissues. The biocompatibility and ability to create functionalized bioconjugates make gold nanoparticles (AuNPs) the perfect candidate for the creation of such structures [1].

The work presents a comparison of the antioxidant activity of catalase immobilized on AuNPs surface by two methods. The first involves protein adsorption directly on the nanoparticles surface. The second is based on the chemical bonding of the enzyme, through the specific binding between the imidazole histidine groups of His-tag-catalase and Ni<sup>2+</sup> ion, complexed by the nitrilotriacetic acid residue present on the surface of AuNPs (NTA-linker). The use of NTA-linker makes it possible to immobilize catalase on nanoparticles without losing its enzymatic activity.

Scientific work supported by National Science Centre of Poland project number 2013/09/B/NZ7/01019 and by University of Lodz, Subsidy for scientific research contributing to the development of young researchers and PhD students, project number: B1711100001603.02.

1.Ranoszek-Soliwoda K., Czechowska E., Tomaszewska E., Celichowski G Kowalczyk T., Sakowicz T., Szemraj J., Grobelny J. Catalase-Modified Gold Nanoparticles: Determination of the Degree of Protein Adsorption by Gel Electrophoresis // Colloids and Surface B: – 2017 – accepted.

## **On the nature of the liquid phase of the metal-containing nanocomposite**

**Kalinichenko K. V.<sup>1</sup>, Nikovskaya G. N.<sup>1</sup>, Kosorukov P. A.<sup>2</sup>**

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In our previous investigations we developed the “green” biocolloid process of conversion of sewage sludge (from municipal waste water treatment plant) into nanocomposite fertilizer [1–3]. This process based on initiation of heterotrophic sludge microbial activity with alkaline vector of metabolism, bioleaching of excess of toxic heavy metals to appropriate level for plant nutrition. The final products of the bioconversion process are solid phase (nanocomposite fertilizer) and liquid phase (supernatant) which contains heavy metal compounds, aminoacids, vitamins etc and can be serve as a potential source of nutrients for creation of artificial soils on the base of acrylic hydrogels.

The objective of this work was to study the nature of the liquid phase and its impact on plant growth.

The supernatant was investigated by dynamic light scattering (Zetasizer Nano S) and X-ray analysis.

It was established heavy metals (Cu, Fe, Zn, Mn, Co, Pb, Ni, Cr, Sr) in the liquid phase are presented in the form of nanosized (50–100 nm) hydroxycarbonate complexes which are eco-friendly and stabilized microbial polysaccharides.

Application of the supernatant, which was incorporated into acrylic hydrogel, provided a significant increase in plant yield.

1. Kalinichenko K. V., Nikovskaya G. M., Samchenko Yu. M., Ulberg Z. R. Gel nanocomposites with immobilized bioelements for plant nutrition // In: Nanophysics, Nanophotonics, Surface Studies and Applications, 2016. – P. 439–449.
2. Kalinichenko K. V., Nikovskaya G. N. Principles of municipal sewage sludge bioconversion into biomineral fertilizer // Int. J. of Chem., Mat. Sci. and Eng., 2014. – 8, No 1. – P. 5–7.

**Photodynamic activity of methylene blue, functionalized  
by gold nanocarriers against mouse melanoma B16 *in vitro***

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Melanoma is a malignant tumor that is resistant to chemo- and radiotherapy. But as cell damage mechanism of photodynamic therapy (PDT) differs from the cell damage caused by abovementioned cancer treatment methods, we assumed that PDT can be more successful against melanoma. Methylene blue (MB) was chosen as a photosensitizer, since this dye has high affinity for melanin and selectively accumulates in melanin-containing cells [1].

In our study mice melanoma B16F10 cell line was used as a model object. It was shown that MB alone in concentrations less than 10 µg/ml did not cause mortality of melanoma cells. At the same time, after irradiation of cells, that was preincubated with MB in this concentration, with a semiconductor laser ( $\lambda = 660$  nm, dose = 12 J/cm<sup>2</sup>), melanoma cell mortality reached 70 %.

To enhance the photodynamic damage of melanoma cells, we used a nanotechnological approach. Gold nanospheres with the diameter of 15 nm, prepared by the citrate method and stabilized by polyvinyl pyrrolidone, (GNP) were used as nanocarriers for the photosensitizer. As singlet oxygen is one of the main active species that generates during PDT, we have determined the optimal MB-GNP ratio for its maximal production, which was equal to 1:5 respectively. Therefore, in our further experiments we used a composite photosensitizer containing 4 µg/ml of MB and 20 µg/ml of GNP. In a result, functionalization of MB by GNP almost twice increased photodynamic activity of this dye. Based on the data obtained it can be asserted that MB-GNP nanocomposite can effectively eliminate pigmented mouse melanoma cells.

1. Link E. M., Brown I., Carpenter R. N., Mitchell J. S. Uptake and therapeutic effectiveness of 125I- and 211At-methylene blue for pigmented melanoma in an animal model system // Cancer Res., 1989. – Vol. 49, N 15. – P. 4332–7.



## Diazafluorene as 1,3-dipole in reactions with conjugated systems of alkenes functionalized electrophilic groups

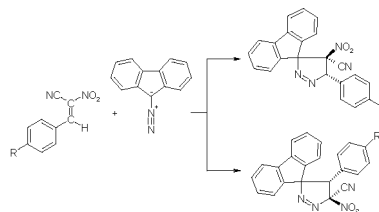
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The reaction between alkenes and diazafluorene (as 1,3-dipole) are known from the beginning of 20<sup>th</sup> century [1]. In the course of 1,3-dipolar cycloaddition  $\Delta^1$ -pyrazoline systems are formed. This type of reaction are realized under mild conditions and provide to products with high yields. The products are used as bioactive compounds, for example in medicines and pesticides [1, 2].

In present work, we prepared compounds functionalized electrophilic group via 1,3-dipolar cycloadditions between diazafluorene and homogenous series of (E)-2-aryl-1-cyano-1-nitroethenes. It was found, that create a two regioisomeric adducts are also possible. These adducts are presented on Scheme 1 [3].



**Scheme 1.** Theoretically possible paths of reaction between diazafluorene and (E)-2-aryl-1-cyano-1-nitroethenes

1. Staudinger H., Gaule A. // Chem. Ber., 1916. – **49**. – P. 1959.
2. Młostoń G., Urbaniak K., Linden A., Heimgartner H. // Tetrahedron Lett., 2009. – **65**. – P. 8191–8196.
3. Jasiński R., Kula K., Kacka A., Mirosław B. Unexpected course of reaction between (E)-2-aryl-1-cyano-1-nitroethenes and diazafluorene: why is there no 1,3-dipolar cycloaddition? // Monatsh. Chem., 2017. – **148**. – P. 909–915.

**Nanostructure-nanochemical processes  
in peloid sediments with biogeocoenosis participation**

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It was studied the microbiological influence of biogeocoenosis on colloid-chemical nanostructure-nanochemical transformations of sulfide clay peloids (therapeutic muds). Samples with unique therapeutic properties containing montmorillonite and glauconite as the main clay nanostructured components, were studied. Modeling of their influence on biocolloid and therapeutic properties was realized on samples of natural bentonite of Dashukovka deposit and glauconite of Satanovka deposit (Ukraine); physicochemical and biomedical properties and their changes under the influence of biogeocoenosis micro-organism metabolic products – using rheological methods. It's shown for the first time, that such changes correlate with nanostructure-nanochemical transformations of clay minerals, which are respectively interrelated with changes of peloid therapeutic properties.

It is shown that researched clays due to their nanostructural features, peculiar microelement composition and high ion exchange and adsorption properties are effective not only in peloid composition, but also in per se form. Their use provides therapeutic and prophylactic effects due to ion exchange and adsorption organism detoxification, providing anti-inflammatory and immunodeficient effect on it. Results of experimental researches on laboratory animals show that bentonite is the most perspective in the treatment of gastric ulcer and hepatitis, and glauconite – in the treatment of dexamethasone arthrosis and endogenous intoxication.

1. Prokopenko V. A., Kovzun I. G., Ulberg Z. R. The creative potential of scientific discovery // Herald of NAS of Ukraine, 2014. – N 10. – P. 52–61.
2. Panko A. V., Kovzun I. G., Ulberg et al. // Springer Proc. in Physics, 2016. – **183**. – P. 163–177, DOI 10.1007/978-3-319-30737-4\_14.
3. Nikipelova E. M. // Odesa National University Herald. Chemistry, 2014. – **3**. – P. 70–75. DOI 10.18524/2304-0947.2014.3(51).40405.

### **Innovative recovery of oxidation enzymes by adsorption on Alumina supports**

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Enzymes are the biocatalysts of the living world, but their properties render them also exploitable in many applications that range from industrial catalysis to therapeutics, including synthetic and pharmaceutical chemistry, wastewater bioremediation, fabrication of high performance biosensors, among others [1–3].

The use of enzymes, however, is limited by their recovery since this aspect plays a significant role in the evaluation of the cost of the biocatalytic processes, therefore several methods have been proposed for their immobilization on stable supports. This study investigates the possibility of using different phases of nano-alumina for enzyme capture and reuse.

Alumina nanoparticles were synthesized in the  $\gamma$  and  $\theta$ - $\delta$  phases with different shapes starting from boehmite and dawsonite thermally calcined at 500 and 1000 °C respectively [4] and tested as adsorbent of commercial soybean peroxidase.

The alumina samples were characterized by thermogravimetric analysis, specific surface area, X-ray powder diffraction, scanning electron microscopy, zeta-potential and Fourier transform infrared spectroscopy.

The kinetic of recovery was evaluated in different experimental conditions (enzyme dosage, pH and temperature, presence of buffer) indicating that the supports can easily capture the enzyme which can be almost completely released for a subsequent cycle of reaction.

1. Marchis T., Cerrato G., Magnacca G., Crocellà V., Laurenti E. Immobilization of soybean peroxidase on aminopropyl glass beads: Structural and kinetic studies// *Biochem. Eng. J.*, 2012. – **67**. – P. 28–34.

2. Torres J. A., Nogueira F. G. E., Lopes J. H., Tavares T. S., Ramalho T. C. Novel eco-friendly biocatalyst: soybean peroxidase immobilized onto activated carbon obtained from agricultural waste// *RSC Adv.*, 2017. – **7**, N 27. – P. 16460–16466.

3. Barbosa O., Ortiz C., Murcia A. B., Torres R., Rodrigues R. C. Strategies for the one-step immobilization!purification of enzymes as industrial biocatalysts // *Biotech. Adv.*, 2015. – **33**. – P. 435–456.

4. Morterra C., Magnacca G. A case study: surface chemistry and surface structure of catalytic aluminas, as studied by vibrational spectroscopy of adsorbed species // *Catal. Today*, 1996. – **27**, N 3–4. – P. 497–532.

**Bioactive glasses doped with salicylic acid****Szalkowska M.<sup>1</sup>, Łukowiak A.<sup>2</sup>, Krzak J.<sup>1</sup>, Babiarczuk B.<sup>1</sup>**<sup>1</sup>*Department of Mechanics, Materials Science and Engineering, Wrocław University of Science and Technology, Wrocław, Poland.**E-mail: marta.szalkowska@pwr.edu.pl*<sup>2</sup>*Institute of Low Temperature and Structure Research, PAS, Wrocław, Poland.*

Bioactive glasses are biomaterials often used in an implantology [1]. Sol-gel bio-glasses, due to the low temperature condition of synthesis, are good carriers of active compounds, especially such with pharmacology properties e.g. ascorbic acid, salicylic acid and others [2, 3, 4]. This organic compound is used in medicine as a disinfectant and as an ingredient in medicines for acne. However, the most important use of salicylic acid is for a production of acetyl-salicylic acid (aspirin).

Salicylic acid functionalized silica-based glasses were synthesized by the sol-gel method. Addition of an active compound was possible due to chemically inert oxide matrix and resulted from the lack of negative reactions between the substrates. Bioactive glasses were prepared in powder form in a basic medium, and as a precursor was used tetraethoxysilane (TEOS). For received powder materials spectrophotometric measurements were performed. Information on the chemical structure was obtained through Raman and FTIR spectra. The presence of salicylic acid in the silica matrix was confirmed by absorption measurements. Received data indicate to a successful functionalization of sol-gel oxide matrices by the salicylic acid.

1. *Arcos D., Vallet-Regi M., Sol-gel silica-based biomaterials and bone tissue regeneration // Acta Biomater*, 2010. – **6**. – P. 2874–2888.

2. *Krzak J., Borak B., Łukowiak A., Donersz-Sikorska A., Babiarczuk B., Marycz K., Szczurek A., Advancement of Surface by Applying a Seemingly Simple Sol-gel Oxide Materials // Chapter in Advanced Surface Engineering Materials (Ashutosh Tiwari, Rui Wang, Bingqing Wei, eds.), Scrivener Publishing LLC and John Wiley & Sons, Inc, 2016.*

3. *Marycz K., Smieszek A., Grzesiak J., Donersz-Sikorska A., Krzak J., Application of bone marrow and adipose-derived mesenchymal stem cells for testing the biocompatibility of metal-based biomaterials functionalized with ascorbic acid // Biomed. Mater.*, 2013. – **8**. – P. 1–12

4. *Kornicka K., Babiarczuk B., Krzak J., Marycz K., The effect of a sol-gel derived silica coating doped with vitamin E on oxidative stress and senescence of human adipose-derived mesenchymal stem cells (AMSCs) // RSC ADV*-2016. – **6**. – P. 29524–29537.

## Conjugates of silver nanoparticles and plant extracts for dermal applications

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Tannins (polyphenols and flavonoids) that exhibit reducing properties and can be used in nanoparticles synthesis are produced by plants tissues for defense. Chemically, tannins are phenolic derivatives. Due to their structure and reactivity they are divided into two groups: hydrolysable and condensed. Tannins from the first class are composed of sugar molecules combined with gallic acid molecules by ester bonds. Second group is based on non-hydrolysable derivatives of flavonoids.

The synthesis of silver nanoparticles with plant extracts has been known for many years. However, it should be kept in mind that the controlled nanomaterials preparation requires the development of extraction and purification procedure of selected natural compounds fractions. Monodisperse nanoparticles of the desired shape and size can be obtained only by the controlled synthesis including such parameters as the molar ratio of the reagents, temperature and duration of the reaction.

This work presents the synthesis of silver nanoparticles (AgNPs) using grape seed (*Vitis vinifera*) and cacao beans (*Theobroma cacao*) extracts. Monodisperse spherical nanostructures were obtained by introducing the additional reducing agent - sodium citrate. The colloids were characterized by UV-Vis spectroscopy and dynamic light scattering technique, while the shape and size of the AgNPs core were determined using scanning transmission electron microscopy. Final conjugated materials were tested as potential skin healing aids.

*This work was co-financed by the NCN project No. UMO 2014/13/B/NZ5/01356 and by University of Lodz, Subsidy for scientific research contributing to the development of young young researchers and PhD students – B1711100001603.02.*

**Spectroscopic study of ordered hybrid complexes  
formation between dye aggregates  
and  $\text{LnVO}_4\text{:Eu}^{3+}$  ( $\text{Ln} = \text{Y, Gd, La}$ ) nanoparticles**

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Recently, nanoparticles (NPs) of different types have attracted great attention in the new rapidly developing field of nanomedicine. Specific types of inorganic NPs can be used as a nanoscale platform for targeting molecules and drugs. In recent years some NPs, i.e. rare-earth doped orthovanadate NPs have revealed high biological activity (oxidative stress prevention, anti-inflammation and neuroprotective activity, antitumor effect) that attracts a lot of interest to these objects as a platform for design of multi-functional drug with the synergetic effect.

The present study is devoted to the establishment of mechanisms of interaction of organic molecules with inorganic nanoparticles based on Ln ( $\text{Ln} = \text{Gd, Y, La}$ ) vanadate and hybrid complexes inorganic nanoparticles/organic molecules with living cells. Spectroscopically was shown that adding cationic dyes to aqueous solutions of inorganic NPs results in the adsorption of dye molecules on the NPs near-surface layer and, in some cases, their ordered aggregation and formation of complex inorganic nanoparticles/organic molecules. It has been found that the pattern and degree of the dye aggregation in dyes/NPs hybrid complexes could be governed by the NPs size and form-factor. The dye aggregate structure has been analyzed within the Kasha and McRae exciton model framework.

For the first time, using a microspectroscopic technique we demonstrate the JC-1 aggregates/NPs complex accumulation within the hepatocyte nucleus region in vitro experiment rather than a typical JC-1 specific accumulation in cell mitochondria. Inorganic NPs are promising nanoscale carriers for the transport of organic molecules into a living cell.



## **Session 2**

### **Nanocomposites and Nanomaterials**

## Unconventional phase transitions in a flat-band quantum Heisenberg antiferromagnet

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We consider the spin-1/2 antiferromagnetic isotropic Heisenberg model on a bilayer honeycomb lattice in the presence of an external magnetic field. We also include an interlayer frustration term. First, we study the case of ideal frustration, when the nearest-neighbor intralayer interactions and the frustrating interlayer interactions are of the same strength. In this case, a completely dispersionless (flat) magnon band may become the lowest-energy one and the localized-magnon picture [1] can be used to examine the system at hand. In the vicinity of the saturation field, we map the low-energy states of the considered quantum system onto the spatial configurations of hard hexagons on an auxiliary honeycomb lattice and face a much simpler problem of classical statistical mechanics. It allows us to study the low-temperature thermodynamic properties and find the finite-temperature order-disorder phase transition driven by a magnetic field, which corresponds to the ordering of localized magnons on the auxiliary bipartite honeycomb lattice. The phase transition belongs to the two-dimensional Ising model universality class. Next, we investigate the case of the small deviations from the ideal frustration geometry, when the flat band acquires a small dispersion. We construct an effective model which is a (pseudo)spin-1/2 XXZ easy-axis Heisenberg model on the auxiliary honeycomb lattice in a magnetic field directed along  $z$  axis. The effective model exhibits a spin-flop transition which is also present in the initial frustrated quantum system with the isotropic Heisenberg exchange coupling.

Our study may have some relation to experiments on  $\text{Bi}_3\text{Mn}_4\text{O}_{12}(\text{NO}_3)$  in a magnetic field. Further details can be found in Ref. 2.

1. O. Derzhko, J. Richter, and M. Maksymenko // *Int. J. Mod. Phys. B*, **29**, 1530007 (2015).

2. T. Krokhmalskii, V. Baliha, O. Derzhko, J. Schulenburg, and J. Richter // *Phys. Rev. B* **95**, 094419 (2017).

## Industrial production of nanocomposite materials

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The last decade of very active develops direction of applied nanotechnology, namely the development and improvement of technologies for a variety of nanocomposite materials for consumer goods. Physical and mechanical properties of structural materials depend on each stage of the process. Getting a high physical and chemical characteristics uniformity depends on the uniform components distribution in the bulk polymer. Therefore, the mixing step is one of the most important in the processing of polymers. A new promising direction for the implementation of this process is using of combined or screw-disc extruders that combine the advantages of both screw and disc machines, providing: high plasticizing and homogenizing power, high degree of mixing, high productivity, possibility of the complex profile products obtaining. Another technical feature of the design is the using of physical fields. The influence of permanent physical field causes displacement and orientation of macromolecules. As a result, formed crosslinked anisotropic structures drawn perpendicular to the direction of the field lines field. This leads to streamlining structures and macromolecules and sealing filler in epoxy composites.

Samples of composites were subjected to hardening under normal conditions, and under the influence a constant magnetic field with intensity  $H = 2 \cdot 10^5$  A/m or constant electric field tension  $E = 1.5 \cdot 10^4$  V/m for 24 hours and the temperature of 293–297 K. Created polymeric composites subjected to temperature stabilization at  $333 \pm 2$  K within 24 h, after which the sample was considered ready for research.

It was found, high quality mixing in these machines driven by circulation flows arising in the working gap, making the profile octahedral deformation shifts repeatedly changes its direction, causing an increase in the interface and change its orientation. As a result, of the research programs have been established, which can be used for determination the quality of polymer composition mixing.

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### Isotopic effect in thermal expansion of organic superconductor $\kappa$ -(D<sub>4</sub>-BEDT-TTF)<sub>2</sub>Cu[N(CN)<sub>2</sub>]Br

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Low-dimensional organic molecular conductors and magnetic materials are a new type of conductive compounds, which are characterized by a delicate balance between the various types of electronic instabilities [1–2]. Their study yielded some interesting results in various areas of solid state physics (metal-insulator and metal-superconductor transitions due to electron correlations, nesting and reconstruction of Fermi surface with low-dimensional characters, drastic changes in transport properties induced by a magnetic field, the angular magnetoresistance oscillations through interlayer coupling, etc.)

Linear thermal expansion coefficient (LTEC) of single crystal  $\kappa$ -(D<sub>4</sub>-BEDT-TTF)<sub>2</sub>Cu[N(CN)<sub>2</sub>]Br was studied across the crystal layers in the temperature range 2–290 K using the method of precise capacitive dilatometry. Below T<sub>c</sub> = 11,6 K the LTEC of the sample had a small negative value, which is apparently due to the transition from the paramagnetic metal in the superconducting state. There was a bend of temperature dependence of the LTEC, which shows broad peak around 40 K and can be attributed to the elastic lattice anomaly around the end-point of Mott boundary. A sharp jump in the LTEC values and hysteresis was observed in the area of T<sub>g</sub> ~ 75–77 K, what is likely explained by the transition in a glass-like state. The isotope effect in the thermal expansion is discussed, which manifested itself in a shift of the phase transitions in comparison with fully deuterated BEDT-TTF sample.

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## **Production of hydrogen by ethanol steam reforming over Co/HAp catalysts**

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Hydrogen is defined as energy carrier for future due to it burns without emitting any greenhouse gases [1]. Nowadays, about 95 % of hydrogen is obtained by steam reforming of natural gas. The main component of natural gas is methane and production of hydrogen in this way causes the atmospheric pollution. One of alternatives can be ethanol steam reforming ( $\text{C}_2\text{H}_5\text{OH} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2$ , SRE). Bioethanol offers environmental friendly production of hydrogen since the  $\text{CO}_2$  produced is consumed for biomass growth [2].

In presented study, the catalytic activity of calcium hydroxyapatite supported cobalt nanoparticles for hydrogen production via SRE was investigated. Co loaded hydroxyapatite catalysts were prepared by incipient wetness impregnation. The catalytic process was conducted at 500 °C under atmospheric pressure using a  $\text{H}_2\text{O}:\text{C}_2\text{H}_5\text{OH}$  molar ratio of 6:1.

Catalytic measurements showed that main reactions over Co/HAp catalysts were incomplete steam reforming and dehydrogenation of ethanol. The occurrence of these reactions was assigned to dehydrogenation properties of support and presence of  $\text{Co}^{2+}$  ions and metallic Co. It was also found that the pre-reduction step decreased the hydrogen yield over Co/HAp samples. The best catalytic properties in terms of ethanol conversion and hydrogen yield showed 5%Co/HAp sample [3].

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## **Magnetic static and dynamical properties of triangular dots arrays**

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Magnetic and magnetodynamic properties of nanomagnetics are of great interest now due to their potential applications for information recording and processing. The simplest systems for the dynamics analysis are nanoellipsoids due to homogeneous distribution of magnetization and internal fields inside them. But from the applications point of view non-ellipsoidal elements are much more attractive.

Here we present results of theoretical and experimental investigations of magnetic and magnetodynamical properties of triangular dots arrays. The nickel dots used in the experiments have 270 nm side and 70 and 130 nm height. The interdot distance was pretty large (~540 nm) to neglect magnetostatic interaction between the dots.

Ferromagnetic resonance spectra of triangular dots was recorded at room temperature using Bruker ELEXSYS E500 electron spin resonance spectrometer operating at 9.87 GHz. The magnetic field was perpendicular to the array plane. Three resonance lines observed for both samples justify the excitation of standing spin waves with different wave vectors in the sample plane. A different behavior of intensity of these modes is observed for 70 nm and 130 nm height dots arrays.

A demagnetizing factor of a regular triangular prism was first theoretically calculated. A dependence demagnetizing field on form factor has been analyzed.

A general expression for the frequency of standing spin waves in regular triangular prism nanoparticles was derived.

## **Novel heating element based on polymer nanocomposites for resistance welding of plastics**

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Resistance welding is one of the most popular welding techniques for thermoplastics nowadays. This technique uses electrically resistive implant sandwiched between the bonding surfaces of the laminates to provide the necessary heat to the joint. When the current flows through the heating element, the heat generated according to the Joule's Law.

Present work describes a new method of the resistance welding of thermoplastic polymers using electroconductive heating element. The heating elements were prepared by incorporation of carbon black (CB) into high-density polyethylene (HDPE) matrix with different variety of volume fraction of the conductive fillers [1].

To evaluate electroconductive properties of the heating elements, they were tested by passing current through it with various values of input voltage [2]. Received information served as an indicator of maximum temperature that can be achieved on specified voltage.

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## Reactive ball milling as the efficient synthesis route of Mg-based composites for hydrogen storage

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Last decades of research in the field of new materials for hydrogen storage were directed to a large degree towards magnesium and Mg-based alloys, which can reversibly store  $\sim 7.6$  wt% of hydrogen. Such sorption capacity combined with low cost suggests that magnesium and its alloys may have advantages in the systems for hydrogen storage [1]. However, the cyclic stability of these materials and their performance at mild temperature conditions are far from satisfactory [2]. Hydrogenation / dehydrogenation properties of the Mg-MgH<sub>2</sub> system can be improved by mechanochemical treatment of magnesium with the addition of transition metals (TM). In this study the influence of TM additives on the room temperature (RT) hydrogen absorption characteristics of nanocomposites based on magnesium, prepared by reactive ball milling under hydrogen in a high energy planetary mill, was explored. On the base of calculated values of the Gibbs free energy for reaction of hydrogen absorption ( $\Delta G < 0$ ) it can be concluded that hydrogenation reaction could thermodynamically proceed at room temperature, which was experimentally confirmed for all of the studied composites. Comparative analysis of the Mg-Ti, Mg-V and Mg-Nb systems makes it possible to establish that the most effective additive facilitating hydrogen uptake at RT is vanadium. It provides the degree of conversion into hydride phase  $\alpha = 0.86$  for the first minute of hydrogenation. In contrast, additives of Nb and Ti provide only  $\alpha = 0.62$  and  $0.36$ , respectively, indeed after 30 min of exposure.

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## Highly efficient photocatalytic conversion of solar energy to hydrogen by core-shell heterojunction nanorods

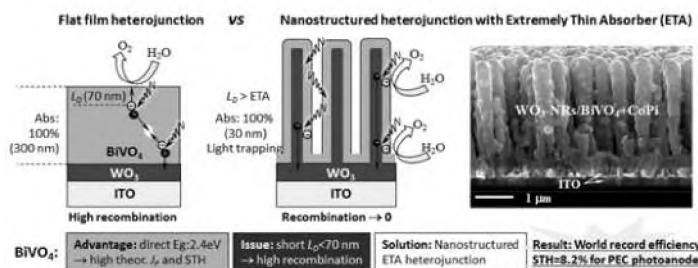
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BiVO<sub>4</sub> is one the most promising photocatalytic materials for water splitting with moderate and direct bandgap of 2.4 eV and high theoretical solar-to-hydrogen conversion efficiency (STH) of 9.2 %. Unfortunately, BiVO<sub>4</sub> has a carrier diffusion length  $L_D$  of only 70 nm, shorter than the optical absorption thickness, that results in high recombination of photocarriers in the film and drop of the photocurrent ( $J_p$ ). I will demonstrate how nanostructured WO<sub>3</sub>/BiVO<sub>4</sub> heterojunction with extremely thin absorber (ETA) BiVO<sub>4</sub> layer (thinner than the  $L_D$ ) avoids recombination losses and achieves almost theoretical  $J_p$ , thus leading to the world record STH of 8.2 % in a water splitting photoelectrochemical cell (PEC) [1, 2]. I will also generalize conceptual advantage of the ETA structure in photocatalysis.



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## **Frustrated quantum Heisenberg antiferromagnets around the localized-magnon paradigm**

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We consider the spin-1/2 antiferromagnetic Heisenberg model on several frustrated one- and two-dimensional lattices with almost dispersionless (almost flat) lowest magnon band in the presence of a magnetic field. The aim of our study is to develop a systematic theory of the low-temperature high-field properties of the models at hand. For these systems we construct the low-energy effective Hamiltonians which are much simpler than the initial ones. For this purpose, we apply the standard strong-coupling perturbation theory and a localized-magnon approach which is valid in a wider range of parameters [1]. To analyze the region of the applicability of the obtained effective Hamiltonians we perform extensive exact-diagonalization calculations and compare them with the results for the initial models. We examine the constructed effective models to explain some properties of the frustrated quantum Heisenberg antiferromagnets in the regime of high magnetic fields and low temperatures.

Furthermore, we apply our analysis to the natural mineral azurite  $\text{Cu}_3(\text{CO}_3)_2(\text{OH})_2$ , the magnetic properties of which can be explained within the spin-1/2 antiferromagnetic Heisenberg diamond spin-chain model with slightly dispersive lowest magnon band. Our theoretical predictions may be of interest for interpreting the high-field low-temperature measurements for azurite [2].

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## **Nanostructured 2D hybrids for photovoltaic and lasing devices manufactured by sol-gel methods**

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Studies on the fabrication of sol-gel optical materials for photovoltaic devices and (or) planar optical waveguide are continuously caring attention over the years because this materials have numerous applications in the field of microelectronics and optoelectronics. However, for oxides many difficulties have to be faced to obtain defect-free, high fidelity, structurally stable patterned films for application in devices. We studied all factors influence on the characteristics of thin hybrid film which would help to tune the quality of mesoscale patterned surface and developed the self-assembled technology based on the sol-gel method to fabricate of high-quality hybrid nanocomposite films using network-forming oxides such as silica or titanium [1]. Preliminary results show that these photosensitive nanostructured films demonstrate nonlinear optical response under excitation of optical pulses of nanosecond duration [2]. The ability of ultrafast excited-state dynamics of composite films containing Rh6G was examined for their potential use as the photonic layer in an all-optical switching device and has obtained the recording of a dynamical grating in a single-pulse regime. Moreover for both films, we observed lasing, which appears as radiation of the central beam that consists from enhanced luminescence and due to the distributed feedback grating of enhancement. Two order reducing the threshold pump intensity and changing the shape of lateral beams under changing TiO<sub>2</sub> matrix instead SiO<sub>2</sub> one is evidence of formation the waveguide amplifier in the TiO<sub>2</sub> film. These results show possibility high-quality lasing of a waveguide that forms the central beam. This work would help on the manufacturing of mesoscale surface patterning of other hybrid films for the perspective application as active optical materials.

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### **Nanosilver surface modification for biological properties formation**

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Nanosilver is the subject of many studies in the context of its use in different fields of science and industry such as optoelectronics, textronics, nanomedicine or biological applications. By controlling the size and geometry of nanostructures (e. g. nanoparticles AgNPs, nanowires AgNWs) and the chemical structure of their surfaces (the presence of stabilizers, organic modifiers or oxide coatings), we can form the properties of the resulting nanomaterials [1].

Work presents the controlled synthesis of AgNPs and AgNWs colloids via chemical reduction method. Afterwards, surfaces of the obtained nanostructures were coated with titanium oxide and tin oxide to form core-shell structures (nanosilver@oxide). The synthesized materials were characterized by the following techniques: DLS, UV-Vis, FT-IR, Raman's spectroscopy and visualized by transmission scanning electron microscopy (STEM). In case of nanoparticles, the influence of pure and modified AgNPs on the growth of plants (*Arabidopsis thaliana*) was investigated. While AgNWs were deposited on the cotton fabrics, and antibacterial properties against *Staphylococcus aureus* and *Klebsiella pneumoniae* were examined according to standards.

The obtained results show great potential of combining the properties of nanosilver with titanium and tin oxides in biological properties formation of final materials.

*This work was supported by University of Lodz, Subsidy for scientific research contributing to the development of young researchers and PhD students, project number: B1711100001603.02.*

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## The formation of nanoscale polygonization substructure in the electric arc coatings of steel 65Г

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The main task of modern engineering is increasing the service life of machine parts and structures. One of the advanced and highly effective way to restore worn parts is to use arc spraying coatings and next pre-recrystallization heat treatment.

Purpose of work is researching of influencing of temperature and time parameters of prerecrystallization heat treatment on the size of electric arc elements of substructure surface.

Arc spraying was conducted at the installation КДМ-2 by electric arc sprayer EM-14M. As the spray material was used wire of 65Г (ГОСТ 9389-75). The heat treatment of samples carried out in an electric furnace – ЧОЛ 1.6.2.0.08 / 9-M1. The hardness  $HV_5$  was determined on the appliance type “Vickers”. The surveys of diffraction patterns was performed on the X-ray diffractometer ДРОН-3.0 in radiation of molybdenum ( $\lambda = 0,071069$  nm).

The obtained samples were heated in a furnace to a temperature of 300, 400 and 500 °C.

The results of the effect of temperature-time parameters of heat treatment: to a temperature of 300 °C maximum hardness values recorded at 4 minutes and endurance is 3.0 GPa; to a temperature of 400 °C is optimal shutter speed 3 minutes with hardness – 3.4 GPa; 500 °C exposure of 1.5 min – 3.1 GPa.

Table 1 shows the results of determining the size of coherent scattering regions (CSR) of samples identified by harmonic analysis. As a standard was used technically pure iron mark Э12 (ГОСТ 3836-83).

**Table 1.** Dimensions CSR of sprayed coating and heat-treated steel 65Г

Treatment	After spraying	300 °C, 4 m	400 °C, 3 m	500 °C, 1,5 m
Size of CSR, nm	121	118	85	99

The influence of temperature and time parameters of pre-recrystallization heat treatment on the hardness and size of the substructure elements obtained coating from a wire 65G were reseached and found that the optimum temperature and time parameters of pre-recrystallization heat treatment include a temperature of 400 °C, holding for 3 minutes, providing nanoscale substructure with size OCD 85 nm.

### Structural peculiarities of ion-conductive organic-inorganic polymer composites

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There is no doubt that lithium ion batteries are one of the most attractive energy storage devices due to their acceptable energy density, environmentally benignity, and long-time cycling. An electrolyte is a key for the performance of a battery and play a critical role in providing high ionic conductivity and transferring mechanical loads. Achieving a clear understanding of the structural and the study of the transport properties is highly important for the development of new effective electroactive materials. Consequently, the research is concerned with hybrid amorphous polymers synthesized basing on epoxy oligomer of diglycide aliphatic ester of polyethylene glycol that was cured by polyethylene polyamine in the presence of lithium perchlorate salt. Structural peculiarities of organic-inorganic polymer composites were studied by differential scanning calorimetry (DSC), wide-angle X-ray spectra, infrared spectroscopic, scanning electron microscopy, elemental analysis, transmission and reflective optical microscopy. Analysis of the results of DSC and wide-angle X-ray diffraction of the composites has shown that all of them are amorphous. At the same time, the results of morphological and structural studies by means of optical and electron microscopes as well as by elemental analysis have revealed the presence of inclusions with sizes from nanometers up to ~ 20 micrometers, probably, of inorganic nature distributed in the polymer matrix. According to the analysis of infrared spectra of the synthesized composites the possible variants of ion-dipole interactions of Li<sup>+</sup> ions with the ether bonds of polyethylene oxide fragments, with OH-groups of the disclosed epoxy rings of diglycide aliphatic ester of polyethylene glycol, with secondary amine groups of polyethylene polyamine, with secondary or tertiary amine groups and the ether bonds simultaneously, are proposed. These hybrid composites represent interest for further investigation and modification as solid polymer electrolytes.

*Acknowledgments:* Matkovska L acknowledges the financial support of the French Ministry of Foreign Affairs, grant No 870734L.

### **Corrosion resistance of ZrO<sub>2</sub> ceramic layers deposited by the sol-gel method on 316L stainless steel in SBF**

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The use of metal implants in medicine entails the contact of metals or metallic alloys with living tissues, the potential release of Fe, Cr, Ni, Mo, etc., metal ions [1] and their accumulation in various parts of the human body. One way in which the corrosive resistance and biological activity of metallic implants can be improved is by covering them with ceramic coatings. Such coatings are a barrier to the release of harmful ions, reduce the risk of inflammatory processes in the body and increase biological activity at the border of the implant-tissue. They can cause the deposition of a layer of hydroxyapatite [Ca<sub>10</sub>(PO<sub>4</sub>)<sub>6</sub>(OH)<sub>2</sub>], which is a natural component of bones and has good osteogenic properties, on the active surface [2].

Thin ceramic ZrO<sub>2</sub> coatings were deposited on a 316L stainless steel substrate by the sol-gel method. Multilayer coatings were obtained from sol containing zirconium(IV) ethoxide (ZrEt) as the precursor butanol as the solvent. Additionally, the sol contained nitric and acetic acids. The sols would be deposited using the dip-coating technique. The sample would be taken out of the solution at a rate of 10 mm/min. The obtained samples would then be exposed to the simulated body fluid (SBF) for 120 days.

The investigations (SEM, EDS, ICP) have shown that the coating of steel 316L with ZrO<sub>2</sub> results in an increase in the barrier properties of the layers in body fluids. The electrochemical measurements and the ICP analyses have confirmed that long-lasting exposure in SBF causes increase in the corrosion resistance of samples coated with ZrO<sub>2</sub> in comparison with uncoated steel 316L and cause increase of apatite ceramics.

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### **Obtaining a homogeneous nanosize film with using an erosive plasma source**

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One of the most widespread methods of film deposition is a plasma spraying method with using erosion sources. The feature of this method is a presence of macro- and micro-inclusions in the resulting coatings, which does not allow to obtain homogeneous nanosize films for using them in nanotechnology. Nowadays, there are methods for filtering microparticles which have some disadvantages such as incomplete removing microparticles or high loss of cathode material during the deposition.

A new method for the deposition of nanoscale homogeneous surfaces has been proposed [1]. This approach consists of destruction microparticles without removing them from the stream. It is based on the use of cylindrical configuration of electrostatic plasma lens for an introduction fast electrons into the volume of dense plasma flow. The fast electrons are generated by the secondary electron emission from the electrodes of plasma lens. Focusing of the plasma flow causes an increase in the density of the plasma flow and speed spraying at any electrode potential. An increase in the pressure of working gas and value of the electrode potential lead to raise in the area of film deposition and its homogeneity. Investigations of sprayed surfaces have been showed the existence of the effect of microparticles destruction with an applied magnetic field in the filter or without it.

Thus, the use of a filter with erosive plasma source allows to obtain nanoscale films of high purity and homogeneity with quite high load factor of material.

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## **Sn induced crystallization of the amorphous Si under laser radiation**

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Sn induced crystallization of amorphous Si under laser radiation was investigated by Raman spectroscopy of thin-film structures Si-Sn-Si. Analysis of the spectra of Raman scattering was used to determine the proportions of amorphous and crystalline silicon phases and the size of Si crystals, formed in a matrix of amorphous Si due tin induced crystallization stimulated by laser radiation. Size and concentration dependency of Si nanocrystals on the power of laser impulses with duration of 150  $\mu$ s as well as 10 ns on wavelength of 1070 nm was experimentally determined and analysed. Thin-film composite “Si nanocrystals in a matrix of amorphous Si” (nc-Si) promises to be a potential material for the next-generation solar cells (SC) based on the quantum dots. It is explained by a number of physical properties that are relevant for the photo-voltaic devices that convert solar energy: quasi-direct band-gap mechanism of light adsorption, dependency of the band gap width on the nanocrystals size, resistance to the Staebler-Wronski effect, suitability for forming on the flexible substrates.

Starting from the intensity of about  $5.5 \times 10^4$  W/cm<sup>2</sup> the size of nanocrystals and the proportion of crystalline phase increases with increase in the power of the laser light. Particularly, increasing the power of radiation from  $(5.5$  to  $7.8) \times 10^4$  W/cm<sup>2</sup> (i. e. by 42 %) leads to the increase in the nanocrystals size from 1.5 nm to 5.0 nm (i. e. by 230 %).

These results confirm the findings of a recent paper [6] on the impact of radiation intensity on the amount and concentration of the crystals in the metal-induced crystallization (MIC) in the structures of Si-Sn-Si under the action of persistent laser radiation. Such kind of the impact has a threshold nature in the area of  $5 \times 10^4$  W/cm<sup>2</sup>. It can be linked, for example, to reaching the melting temperature of the Sn layer in the analysed structures. According to [7], transition into the liquid state is the necessary condition for MIC of the amorphous Si.

It is distinctive that with increase in the intensity from  $(5$  to  $8) \times 10^4$  W/cm<sup>2</sup> (and therefore in the temperature of the impact area of the laser beam) increase in the crystalline phase volume is much slower than the increase in the nano-

crystals size, although the crystal volume  $\sim L^3$ . This means that only a certain part of the original nanocrystals serves as the precipitation nuclei of the Si solution in Sn, and most of them dissolve, because they are smaller than the critical nucleus.

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## **Ferromagnetic resonance in NiMnCoSn epitaxial films with nanotwin structure**

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Magnetic shape memory alloys (MSMA) are of great interest now both from fundamental point of view and for their possible application. A lot of new physical effects related to martensitic transformation have been discovered recently in these materials: giant change of their size under the action of magnetic field, magnetic superelasticity, ordinary and inverse magnetocaloric effect, giant magnetoresistance, bias exchange, etc.

This work is devoted to the investigation of evolution of magnetic and magnetoresonance properties of epitaxial NiMnCoSn films deposited on MgO (001) substrates in 100–400 K temperature range. It has been shown experimentally that these films undergo the martensitic transformation near the room temperature from cubic high temperature austenitic phase to orthorhombic low temperature martensitic one. The characteristic feature of ferromagnetic resonance spectra of this compound in martensitic state is the presence of well field separated three resonance lines. The analysis of structural, magnetic and magnetoresonance properties of the samples does not allow ascribing the appearance of these lines due to formation of phases with different magnetic parameters. It cannot be also explained in terms of spin wave modes formation. Meanwhile the analysis of magnetic data shows a presence of antiferromagnetic interaction in the system.

The appearance of three resonance lines was explained in the frame of following model: ferromagnetic exchange interactions inside martensite twins and antiferromagnetic on the twins boundaries. As a result of such interactions three resonance modes should be observed like it takes place in usual antiferromagnetics, but the modes splitting in our case is much less due to the localization of antiferromagnetic interaction.



## Resistive ethanol vapor sensors based on polyethylene glycol/carbon nanotubes composites

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A highly efficient sensors to organic solvents based on polymer composites has wide application in medicine, industries, environmental monitoring and other fields. Polymer composites filled with carbon nanotubes (CNT) arouse significant scientific interest due to such advantages as easiness of sensor production, comparative cheapness and high performance.

The sensing materials in our study were based on polyethylene glycol ( $M_w = 10000$ ) (PEG) and CNT composites. The composites with 1.5 % CNTs shows the best response.

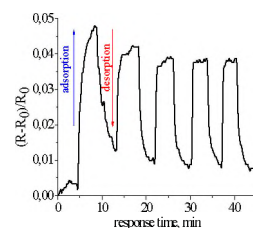


Fig. 1. Resistance response of PEG/CNT sensors in ethanol vapor ( $7 \text{ mg/m}^3$ ).

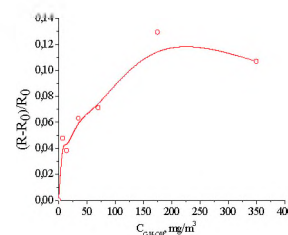


Fig. 2. Relative resistance of PEG/CNT sensor vs. ethanol vapor concentration.

The relative resistance of the sensor at the ethanol adsorption increases during 4–6 min (Fig. 1). And the vapor desorption causes the decreasing of the relative resistance of the sensor during 3–5 min.

Relative resistance of PEG/CNT sensor has exponential growth with the increasing of ethanol vapor concentration from 0.04 to 0.12 (Fig. 2.). The resistance of the sensors at the adsorption of ethanol with concentration from 7 to  $350 \text{ mg/m}^3$  increased to 9.7 kOm.

## Nanostructured GeAsSe chalcogenide glasses: Raman spectroscopy studies

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Chalcogenide glasses (ChGs) due to their unique properties: transparency in IR region, quasistability, numerous photoinduced phenomena, ion-conductivity of doped ChGs serve as a base of their application. ChGs are widely used in versatile technological applications such as infrared optical elements and all-optical switching devices, holography recording media, etc.

This work is devoted to investigation of structural properties of  $\text{Ge}_x\text{As}_y\text{Se}_{100-x-y}$  glasses, where  $x = 0; 2.1; 6.4; 8.5; 10.6$  and  $y = 35.8; 36.6; 37.4$  and  $39.2$  – in the so-called nanophase separation region. Raman spectra of Ge-As-Se samples were measured in the spectral range from 50 to 400  $\text{cm}^{-1}$  at room temperature. Observed bands in the Raman spectra, HH- and HV-polarized Raman spectra of Ge-As-Se samples can be explained in the terms of vibrational modes of binary  $\text{As}_2\text{Se}_3$  and  $\text{GeSe}_2$  glasses. We performed Gaussian deconvolution of obtained Raman spectra that were fitted for a quantitative analysis of their compositional dependencies using home-made software CoRa.

The results of Raman spectra fit showed that the backbones of the studied samples consist of  $\text{AsSe}_{3/2}$  pyramidal units (226  $\text{cm}^{-1}$ ), containing As-As bonds  $\text{As}_4\text{Se}_4$  structural units (245  $\text{cm}^{-1}$ ),  $\text{As}_4\text{Se}_3$  entities (237  $\text{cm}^{-1}$ ), corner- and edge-shared  $\text{Ge}(\text{Se}_{1/2})_4$  tetrahedral units (198 and 213  $\text{cm}^{-1}$ , respectively) and Se-Se-bonds (258  $\text{cm}^{-1}$ ). The bands located in the 100–200  $\text{cm}^{-1}$  region confirm the presence of structural units containing As-As bonds and/or Ge-As vibrations.

Compositional dependences indicate that intensity of the bands corresponding of nonstoichiometric molecular fragments with Ge-related and homopolar As-As bonds is increased with the growth of Ge content. The intensity of the bands corresponding to Se-Se bonds is decreased with higher Ge content.

Thus, Raman data show that Ge-As-Se glasses contain different nanophases whose concentration is changing along chosen compositional cross-section.

*Acknowledgment:* The research was partially supported by the project N 0117U000422 of Ministry of Education and Science of Ukraine.

## Electrical conductivity of PANI-PVDF-MWCNT nanocomposites

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Metals are traditional coating materials for shielding of electromagnetic radiation. Despite of high efficiency the use of metals is associated with operational difficulties, such as a large weight, low resistance to corrosion and complexity of processing. The use of polymer composites with multi-walled carbon nanotubes (MWCNT) can get rid of these problems (drawbacks) and opens new possibilities for creating shielding coatings [1]. This determines the relevance of the study of electrical characteristics of composite materials of polyaniline (PANI) and MWCNT in polyvinylidene fluoride matrix (PVDF).

Relative temperature dependences of resistivity of samples of PANI-PVDF, PANI-PVDF-MWCNT (1 and 15 %), pure PANI, pressed MWCNT were obtained (measured). Based on the comparison of experimental results with theoretical models, we found that these materials have different mechanisms of electrical conductivity. Thus, in the temperature range of 6–300 K samples of PANI-PVDF and PANI-PVDF-MWCNT (1 %) displayed relative temperature dependences of the resistivity, which are characteristic of variable range hopping conduction mechanism (VRH). However, in the case the sample of PANI-PVDF-MWCNT (15 %) VRH conduction mechanism is realized only at temperatures below 24 K. At higher temperatures the temperature dependence of the resistivity is well described by the model of fluctuation-assisted tunnelling (FAT) between metal islands through the thin barrier. Realization of the specific mechanism of the conductivity depends on temperature and sample composition. It should also be noted that the electrical conductivity of the nanocomposites composite material of PANI-PVDF-CNT (15 %) is not a simple sum of the conduction mechanisms of its components.

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### **Thermal expansion coefficient of Al + 1% NTCM nanocomposite**

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The nanocomposite curve contains several dilatometric anomalies having intensities whose variation rates are as a function of temperature. Overall, the thermal expansion coefficient of Al+1% NTCM is comparable to that of conventional aluminum alloys.

Analysis of the dilatogram shows that the appearance temperatures of the different peaks are 80, 150 °C and the third, less intense than the second, at 530 °C. Their origins are different and can be linked to several factors including the catalysts used to obtain the carbon nanotubes and the formations of the amorphous and crystalline phases of the alumina as well as that of the aluminum carbide.

However, the gap between the expansion coefficient values of the conventional aluminum alloys and of the nanocomposite studied are very important. It is considerably lower than that of the conventional aluminum compounds and even of those of the aluminum alloys produced by the various techniques of rapid cooling. Thus, the addition of the CNTs in the matrix is at the origin of a drastic decrease in the thermal expansion coefficient. This important feature may have several origins. Carbon nanotubes produce a refinement of the microstructure. The formation of the  $Al_4C_3$  carbide by diffusion of the carbon in the matrix Al increases the amount of defects. This result is confirmed by Raman spectroscopy. Calorimetric analysis also confirm the presence of anomalies on the DSC curve.

## Impedance spectroscopy of nanopowder systems based on $\text{ZrO}_2$ in a dispersed state

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Nanopowders based on zirconia has a great scientific interest due to a unique combination of physical and chemical properties. The problem of diagnostics of structural-energy state is urgent and requires new methods of solution. Electrochemical impedance spectroscopy (EIS) is one of the most convenient tools for studying of electrophysical properties of the surface of nanoparticles.

The study of electrical properties of surface of nanoparticles by the EIS was the aim of this work.

Nanopowder of  $\text{ZrO}_2 + 3\% \text{Y}_2\text{O}_3$ , compacted by high hydrostatic pressure was the object of investigation. Carbon contacts were applied mechanically. Frequency range is 1Hz- 1MHz.

On Fig. 1 the typical spectrum of the system under study are shown. Two regions with different character of impedance can be distinguished: 1) a fragment of the arc of a circle  $\alpha$  located in the high-frequency region; 2) a straight-line section  $\beta$  in the low-frequency region.

The semicircle  $\alpha$  reflects the capacitive nature of the resistance of the nanoparticle volume. The beam  $\beta$  is associated with electrokinetic phenomena in the interface of the particle-electrode surface. Obtained spectrum is reflect the electrokinetic processes that typical for the system under investigation.

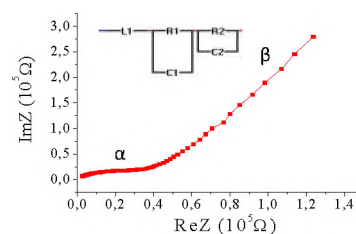


Fig. 1. Typical spectrum of compacted  $\text{ZrO}_2$ -3mol %  $\text{Y}_2\text{O}_3$  nanopowder and its equivalent circuit.

## Synthesis and characterization of ZnSe and ZnSe:Ag nanowires for photovoltaic application

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Synthesis and characterization of semiconductor nanocrystals (NCs) based on cadmium chalcogenides for optoelectronics is a major area of nanotechnology. However, cadmium based nanoparticles are highly toxic and that makes researchers to look in the direction of less toxic materials such as zinc chalcogenides [1]. One of most promising candidates is zinc selenide (ZnSe) characterized by a number of unique physical and chemical properties. For instance, the relatively wide band gap ( $E_g = 2.7$  eV at 300 K) of ZnSe NCs is optimal for converting solar energy into electricity [2].

In this work, the ZnSe NCs are successfully synthesized from two precursors zinc stearate and selenourea in solution of octadecylamine by high temperature method in the presence of argon. Nanoparticles were obtained within 1h at temperature of 150 °C.

ZnSe:Ag nanowires characterized by small diameter about 6–8 nm, a high rate of absorption and green emission. FT-IR shows that on the surface of the nanoparticles are present characteristic groups from octadecylamine, which makes it possible to receive NCs with hydrophobic properties or further surface modification for polymer applications.

*This work was financially supported by National Centre for Research and Development under Lider Program, contract No. LIDER/009/185/L-5/13/NCBR/2014.*

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## Characterization of graphene oxide reduction methods

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Graphene oxide (GO) is an oxidized form of graphene, where the oxygen containing functional groups (hydroxy, epoxy, carboxy and carbonyl) are attached to carbon atoms with sp<sup>3</sup> hybridization. The presence of these groups makes the GO flakes hydrophilic and dispersible in water. However, physical properties of fully oxidized GO can be tuned to those characteristic for pristine graphene by removal of the functional groups from its surface by a simply reduction processes.

Reduced graphene oxide (RGO) can be obtained by chemical, physical and also biological strategies [1]. RGOs obtained by these methods can differ in the amount and type of residual oxygen moieties, number of structural defects and size of sp<sup>2</sup> domains. Such structural differences have major impact on the physical and chemical properties of RGO including its hydrophobicity.

In this work, the chemical reduction of GO and radiolytic reduction of GO are presented. RGOs obtained by the chemical reduction and radiolysis were examined by microscopic and spectroscopic techniques showing that both methods provide comparable results. The reduction was controlled by the process conditions (the time of reduction by ascorbic acid in chemical method, and the dose of irradiation in radiolysis). Finally, the perspectives related to challenges and opportunities in the application and designing of nanocomposites containing GO and RGO are also discussed [2].

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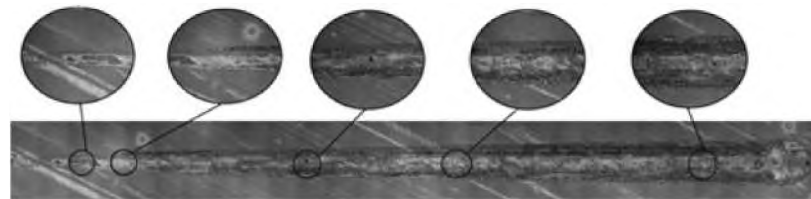
### Adhesion and scratch resistance of sol-gel thin films on polymeric substrate

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Sol-gel thin films are widely used for formation of functional coatings on different substrates. Reactions and deposition process take place in the liquid phase, what allow to form materials with desired properties [1]. However, the particular physico-chemical properties, especially in nanoscale, depends not only on the composition and synthesis parameters but also on the properties of the substrate on which the film is applied [2]. Films deposition on polymeric substrates is difficult due to their low surface free energy, which results in limited wettability and finally adhesion of deposited films [3].

In this work sol-gel  $\text{SiO}_2$  and  $\text{SiO}_2/\text{TiO}_2$  thin films on PET (poly(ethylene terephthalate)) were investigated by the micro-scratch-test measurements, to determine adhesion and scratch resistance of films. The photography of received scratch presented in Fig. 1. shows the different types of resulted failures.



**Fig. 1.** Scratch of the  $\text{SiO}_2/\text{TiO}_2$  coating with different types of failures

*Acknowledgements.* Work created as a result of the research project No. 2016/21/N/ST5/01276 funded by the National Science Centre, Poland.

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## Thermal behavior of high performance nanoporous nanocomposites based on cyanate ester resins and POSS

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In this work, novel thermostable nanoporous nanocomposites based on cyanate ester resin (CER) and epoxycyclohexyl-functionalized polyhedral oligomeric silsesquioxane (ECH-POSS) were synthesized by polycyclotrimerization of dicyanate ester of bisphenol E as well as chemically doped by 0.025–1.0 wt.% ECH-POSS in the presence of 20 wt.% imidazolium tetrafluoroborate [C<sub>12</sub>C<sub>6</sub>Im][BF<sub>4</sub>] ionic liquid (IL) as a porogen, followed by a simple extraction of the IL after complete high temperature CER network formation. Thermal behavior of nanoporous CER/ECH-POSS nanocomposites prepared was investigated by TGA, DSC and DMTA techniques. It was established that the nanoporous films obtained possessed higher thermal stability ( $T_{\text{onset}}$  increase by 30 °C) and increased  $T_g$  (DSC) by ~10–50 °C in comparison with respective CER/ECH-POSS/[C<sub>12</sub>C<sub>6</sub>Im][BF<sub>4</sub>] precursors. It is concluded that the CER/ECH-POSS nanoporous materials are promising materials able to work under extreme conditions (high temperatures, high humidity, corrosive media...).

*Acknowledgements.* The authors gratefully acknowledge the National Academy of Sciences of Ukraine (NASU) and the “Centre National de la Recherche Scientifique” of France (CNRS) for partial financial support through bilateral cooperation project No 26199. They are also indebted to Campus France for providing A. Vashchuk with an Eiffel grant (No 870769C) for a long-term stay at ICMPE.

### **Effect of sputtering and annealing conditions on the structure and properties of FePt-based thin films**

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Improvement of hard disk drives technology requires application of magnetic materials with high magnetic anisotropy and coercivity because of thermal instability problems.  $L1_0$ -FePt nanoscale films are considered the most promising candidates for ultra high density magnetic recording media due to very large magnetocrystalline anisotropy of  $L1_0$ -FePt ordered phase –  $7 \times 10^6$  J/m<sup>3</sup>. Such high magnetic anisotropy constant could provide thermal stability of magnetic medium even at grain size less than 3 nm, leading to maximum possible magnetic recording density. However, after deposition onto room temperature substrates FePt films have a disordered structure with low magnetic properties. High temperature annealing is required for  $L1_0$ -FePt phase formation. Besides ordered phase formation temperature reduction many other aspects should be considered for FePt films industrial application – formation of small  $L1_0$  phase grains with (001) orientation, stabilization of surface roughness as well as coercivity improvement.

The detailed analysis of structural and magnetic properties of FePt-based films depending on the substrate choice, presence of additional layers and compound of annealing atmosphere was conducted. It was shown that drastic increase of films coercivity as well as reduction of ordered phase formation temperature could be reached by Ag intermediate layer introduction into FePt films [1]. Annealing of FePt films in forming gas (Ar+3% $H_2$ ) instead of Ar and  $N_2$  atmospheres leads to suppressing of grains and surface roughness growth [2]. Layered Fe/Pt films deposition onto  $Al_2O_3$  single crystalline substrates and following annealing leads to pronounced (001) texture formation and low-temperature  $L1_0$  phase nucleation, which was not observed using other substrates [3].

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### Spin-dependent scattering in Co/Ni-Cu multilayers under magnetic proximity effect

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Giant-magnetoresistant (GMR) multilayers Co/Cu/Co are well-known to exhibit oscillatory exchange coupling (OEC). OEC was also observed in Co/PM(paramagnetic)/Co systems [1]. Recently the magnetic biasing effect on the PM atoms at the FM(ferromagnetic)/PM interfaces – the so-called proximity effect (PE) – was discussed [2]. Such PE can substantially alter both (i) the effective thicknesses at which the antiferromagnetic peaks of the OEC are observed [1] and (ii) the spin-diffusion length due to enhanced local magnetic moments of PM scattering centers at the FM/PM interfaces.  $\text{Ni}_x\text{Cu}_{100-x}$  binary alloys with low Ni concentrations are of particular interest since at  $x < 30\%$  Ni atoms diluted in Cu are expected to essentially become nonmagnetic [2]. The subject of this study is the influence of PE on magnetotransport in Co/Ni-Cu multilayers.

Here we design a Co/Ni-Cu/Co multilayer system with suppressed PE by incorporating a Cu/Ni-Cu spacer and demonstrate a paramagnetic-to-non-magnetic transition in the integrated Ni-Cu layers. We report a step-like feature on the magnetoresistance vs.  $x$  in the critical concentration interval of  $x = 15\text{--}25\%$  and assign it to Ni in Cu to develop strong atomic magnetic moments and thereby turn into strong PM scattering centers.

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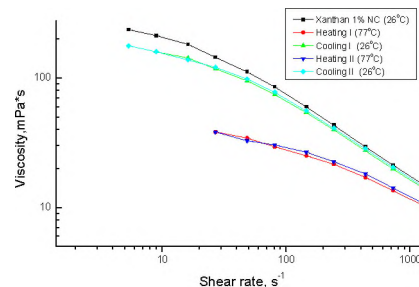
## Rheological properties of xanthan/nanoclay hydrogel

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Xanthan hydrogels are widely used as viscosity regulators and stabilizers for cosmetics, food, and other industrial applications. Such composites work as thickeners and texturizers due to formation of three-dimensional network and polysaccharide order-disorder transitions under change of temperature, concentration or ionic strength of the solution. Addition of the nanofillers can influence on rheological properties of the polysaccharide solution and change the character of fluidity significantly. Another option to govern the composite-hydrogel rheology is temperature change. In this research we investigated influence of several heating/cooling cycles on the fluidity behavior of the xanthan/montmorillonite solution.



**Fig. 1.** Dependence of viscosity of 1%Xanthan/20%nanoclay(w/w) on the repeating heating/cooling

At low concentration (1% of nanofiller) the character of fluidity for composite hydrogel is similar to the pure xanthan hydrogel and represents the shape of the curve of non-newtonian solution. Heating the composite hydrogel over the xanthan conformation transition temperature (60–70 °C) leads to sufficient growth of viscosity with further relaxation to the initial viscosity after cooling as well.

## Magnetopiezoelectric effect in Sm and Nd ferroborates

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We have investigated piezoelectric responses in samarium and neodymium ferroborates. It appeared that the samarium compound demonstrates a giant magnetopiezoelectric effect-the effective PM is increased more than twice in the antiferromagnetic phase and it is suppressed by a magnetic field [1]. The cause of the PME is caused by the combined action of the elastic and electric fields on the orientation of the magnetic vectors in the reference plane (including the spin-flop phase. In general the nature of the MPE effect is alike to magneto-capacitance effect (ME) which is inherent for multiferroics.

The given below results [2] are related to another representative of ferroborate's family – neodymium ferroborate –  $\text{NdFe}_3(\text{BO}_3)_4$ . The main aim of these investigations was to detect the general laws of manifestation of MPE and ME effects in such compounds. It was obtained that despite some quantitative differences, the characteristics of these effects are similar for all easy-plane ferroborates. At fields that exceed the spin-flop one the relative changes of piezomodulus  $\delta e/e$  and permittivity  $\delta \epsilon/\epsilon$  are described by the phenomenological equations:

$$\delta e/e = ab \sin^2 2\varphi/e \chi H^2; \quad \delta \epsilon/\epsilon = 4\pi a^2 \sin^2 2\varphi/e \chi H^2$$

Here  $a$ ,  $b$  are magnetoelectric and magnetoelastic coefficients,  $\varphi$  is angle between magnetic field direction and  $C_2$  axe and  $\chi$  is the magnetic susceptibility. On Fig. 1. it is shown that the linear in  $H^{-2}$  dependence are well fulfilled. From the slope of the approximating straight lines constants  $a$  and  $b$  can be easily determined. For  $\text{NdFe}_3(\text{BO}_3)_4$  at  $T = 1,7 \text{ K}$ ,  $a = 450 \text{ } \mu\text{C}/\text{m}^2$ ,  $b = 8 \times 10^6 \text{ J}/\text{m}^3$ .

Temperature influence was also investigated by DSC, and obtained data were in good correspondence with rheological measurement results.

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# **Session 3**

## **Nanooptics and Photonics**

### **Light-induced LC director freezing on a chalcogenide surface**

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First observations of permanent light-induced director patterning in a transparent liquid crystal (LC) are reported. The patterning was observed in an LC cell with one of the substrates covered with a chalcogenide film. Concentric director ring pattern appears following the irradiation of the chalcogenide surface through the LC layer by a Gaussian beam. The experimental results are explained in terms of the heat transfer from the chalcogenide film to the LC after the light absorption by the chalcogenide film. Heating the LC changes its birefringence according to the spatial intensity distribution of the Gaussian beam. This in turn leads to the spatially oscillating changes of the polarisation state of light in the plane of the chalcogenide film. The oscillating changes of the light polarisation result in producing the light-induced easy orientation axis and the oscillating changes of the anchoring energy. It causes the spatial modulation of the director on the chalcogenide surface and the formation of the concentric ring twist structures in the cell.

## Energy transfer and near infrared emission in $\text{GdVO}_4\text{:Bi}^{3+}$ , $\text{Ln}^{3+}$ ( $\text{Ln}=\text{Nd}^{3+}$ and $\text{Yb}^{3+}$ ) nanophosphors

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Near-infrared (NIR) light-emitting optical materials attract attention because of wide applications as solid state lasers, fibre optical communications, chemical and biological sensing, infrared bioimaging. Additionally, the NIR luminescent lanthanide ( $\text{Ln}^{3+}$ ) nanomaterials can also help in enhancing of a silicon-based solar cell efficiency. The spectral mismatching of incident photons especially the low energy photons ( $\lambda > 1100$  nm) as well as the high energy photons ( $\lambda < 400$  nm) causes thermalization losses in the silicon-based solar cell.

It is possible to obtain of the efficient near-infrared light-emitting material through an increase of a NIR luminescence of  $\text{Ln}^{3+}$  ions by means of three ways: (a) choosing a self-activated host matrix that can transfers its excitation energy to activators like  $\text{Ln}^{3+}$  ions; (b) to incorporate a sensitizer; (c) quantum cutting (QC) and downconversion (DC) by suitable co-doping.

In the present work, in which an energy transfer and a near infrared emission in  $\text{GdVO}_4\text{:Bi}^{3+}$ ,  $\text{Ln}^{3+}$  ( $\text{Ln} = \text{Nd}^{3+}$  and  $\text{Yb}^{3+}$ ) nanophosphors were investigated, the all three ways were used. Gadolinium orthovanadate ( $\text{GdVO}_4$ ) is a well-known self-activated host matrix [1]. The bismuth ( $\text{Bi}^{3+}$ ) ion was used as a sensitizer. Rare earth ions like neodymium ( $\text{Nd}^{3+}$ ) and ytterbium ( $\text{Yb}^{3+}$ ) were chosen because they are well-known NIR luminescence centres. Obtained results demonstrated that  $\text{Nd}^{3+}/\text{Yb}^{3+}$  and  $\text{Bi}^{3+}$  co-doped  $\text{GdVO}_4$  submicro- and nanophosphors might act as a NIR downconversion solar spectral converter [2, 3].

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### Third-order nonlinear susceptibility of ZnO nanoparticles using third-harmonic generation at interfaces

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Bright harmonic nanoparticles (HNPs) allowing all-optical frequency conversion attract considerable attention due to their potential applications in various domains including modern telecommunication systems [1] and bioimaging [2]. Strong light-light interaction at the nanometer scale can indeed benefit to the information and communication technology field for the design of highly compact photonic devices based on nonlinear and quantum optics. Considering this growing interest, dedicated nonlinear optical characterization methods of HNPs are required. In this work, efficiency of the third harmonic (TH) generation of ZnO HNPs under nanosecond laser excitation at 1064 nm was studied with the interface scanning technique [3]. This approach is for the first time used here with a suspension of HNPs after application of a random nanocomposite model. An applied approach demonstrates the high influence of NPs agglomeration on THG efficiency.

An estimated value of effective cubic susceptibility  $\chi^{(3)} \sim 3 \times 10^{-18} \text{ m}^2/\text{V}^2$  for ZnO HNPs of  $\sim 150 \text{ nm}$  mean size obtained by interface scanning was then compared with the one deduced from TH scattering experiments by using the same experimental setup as detailed in [4]. Considering that the orientationally averaged quantities probed by the interface and scattering techniques shows different efficiencies, this work demonstrates that applied techniques can be used for rapid characterization of HNP colloids.

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# **Session 4**

## **Nanoplasmonics and Surface Enhanced Spectroscopy**

### Experiment and modeling of “star-like” plasmonic nanostructures for SERS application

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Surface-enhanced Raman spectroscopy (SERS) is an effective analytical method that is commonly used in diagnostics of substances in chemistry, material science, medicine, biology, pharmacology, ecology, homeland security etc [1].

Star-shaped plasmonic gold nanostructures (NSs) were synthesized by chemical methods for SERS application [2]. Their morphology, absorption spectra and efficiency of the Raman signal enhancement of molecules were investigated.

SEM and TEM studies have shown that obtained NSs possess “star-like” form with core in the centre and cones on its surface. Arrangement of NSs on the surface of SERS substrate is quite dense that causes the formation of so-called “hot spots”, where the intensity of electric field is much higher than its average value, which is caused by superposition of electric fields of nearly placed NSs.

Absorption spectra of obtained NSs have shown intense plasmonic absorption peak with a maximum at 600 nm. It was shown that SERS-substrates with such NSs effectively enhance scattered Raman signal of molecules by using lasers with wavelengths 632 nm, 532 nm as the excitation source. Computer modeling by finite element method calculated the distribution of electric fields near NSs. This helps us to optimize morphological parameters of NSs during their synthesis and deposition on glass substrates for more effective enhancement of the Raman signal.

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### Single molecule detection using silver dendrites in pores of SiO<sub>2</sub> template

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

The template was a porous matrix of silicon dioxide on silicon with pores size of 700–800 nm. The formation of spatially separated dendrites in the pores of the template was performed by immersing of SiO<sub>2</sub>/Si in the aqueous solution of 0.02 M AgNO<sub>3</sub> and 5 M HF for 30 s. Investigation of the enhancement of Raman scattering were carried out on the Ellman's reagent (C<sub>14</sub>H<sub>8</sub>N<sub>2</sub>O<sub>8</sub>S<sub>2</sub>) with concentrations in the range of 10<sup>-4</sup>–10<sup>-15</sup> M. A green laser with a wavelength of 532 nm and a power of 1 mW within the exposure time of 1 s was used in the experiment. Analysis of the obtained data indicates the possibility of detecting ultra-small concentrations (single molecule) of the Ellman's reagent, the detection limit of which was 10<sup>-15</sup> M, and the enhancement factor of the Raman signal reached more than 10 orders of magnitude. Thus, spatially separated dendrites in the pores of the SiO<sub>2</sub> template on silicon are effective plasmon-active surfaces for SERS, which have a record-high sensitivity and can find application in chemo- and biosensors.

## Theory of THz radiation detection in hybrid plasmonic semiconductor structures with 2DEG

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The terahertz plasmonics is the new field of researches and technologies that oriented on study of excitations of plasma oscillations in modern nanoscale heterostructures with purposes of the development of new devices, which operate in the THz frequency range. Recently, it was proposed to use effect of electrically driven plasma instabilities for generation and amplification of THz radiation [1]. Also, plasmonic structures with incorporated metallic grating can be used as detectors of THz radiation. Such structures have great perspectives due to the large effective optical area, possibility of current control of spectral sensitivity. Also, metallic grating plays role of efficient broadband antenna. Theoretical description of the THz detection at the excitations of 2D plasmons was proposed in ref. [2]. Authors considered very simplified model of plasmonic structures and the theory had the lacks from point of view of self-consistency.

We developed a rigorous theoretical approach for calculations of photo-response spectra taking into account radiative decays of plasmons, multilayer geometry of plasmon structure and realistic current-voltage characteristics. Our theory was applied for AlGaAs/GaAs heterostructures with metallic grating with submicron periods. We found that in spectral range of 0.4–1 THz at applied dc electric field of 0.4 kV/cm, photoresponse reaches values of 35 mV. Also, we proposed the recommendations for improvement of THz radiation detectors based on hybrid plasmonic structures with 2DEG.

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**Influence of dielectric film thickness  
on the surface plasmon resonance in the system  
“Au NPs monolayer – dielectric spacer – Al film”**

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In recent years intensively studied layered planar structures containing monolayer of metal nanoparticles and metal screen separated by a dielectric layer (film) [1–3].

The purpose of present work was to study the influence of the thickness of dielectric shellac layer on spectral characteristics of surface plasmon resonance (SPR) in a planar three-layer system: 2D array of Au nanoparticles with a diameter of 90 nm – dielectric shellac film with variable thickness in the range of 3–200 nm – Al film with thickness of 50 nm, deposited on a glass substrate. The extinction spectra of this system were measured. The resulting spectra were peak-fitted by Gauss peak functions. Proceeding from this, we identified the spectral peak of SPR in gold nanoparticles and determined its spectral characteristics. It was obtained that decrease of the thickness of shellac caused the considerable (140 nm) red (low-energy) shift of extinction peak of surface plasmons (SP). As well, the non-monotonic dependences of peak and integral intensities of plasmon extinction peak on shellac film thickness were observed. It was obtained that the maximum extinction is observed at film thickness of 70 nm. Another interesting effect is an appearance in the extinction spectrum, besides the low-energy dipole SP peak, the additional high-energy peak caused by the excitation of quadrupolar SP, occurring when shellac film thickness is less than 30 nm. As the shellac film thickness decreases, the quadrupolar SPR peak red shifts also, but its shift value is significantly less than one of dipole peak. The probability of optical transitions caused by quadrupolar SP increases, while the probability of transitions associated with dipole SP decreases.

Based on the experimental results, we can conclude that the such structures can be used in nanophotonic devices where there is a need for controllable and smooth tuning of spectral position and intensity of the extinction spectrum.

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## **Session 5**

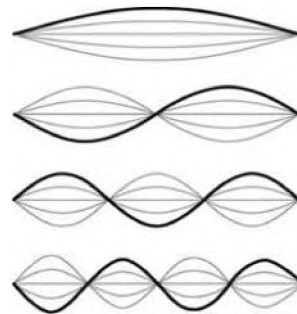
### **Nanoscale Physics**

## Atoms, elementary particles – acoustic waves and experiments with them

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Oscillations of particles make a possibility to create waves. Conducting special experiments allows to get to know more about them. Using oscilloscope with lamp, which interior makes for electrons movement, is an example to state a velocity of sound. It was made in two gases – air and carbon dioxide. Velocity in air was also showed due to standing waves. Standing waves (1) moving in a tube. Carried researches on waves pointed that a sound has not one velocity, but it depends on surroundings. These phenomenons are possible because particles are not standing without move.



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**Possible conditions of increasing the rate  
of the  $\text{SPNH}^+ \rightarrow \text{MCOH}^+$  reaction**

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To date, one of the important goals in nanotechnologies is building electronic devices using single molecules. Photochromic molecules are potential candidates for realization an elemental base of molecular electronics which is developing on the principles of intramolecular electronic processes. One of the the most interesting photochromic molecule is the spiropyran molecule (SP). It can change its structure and properties not only under UV irradiation, also in response to external inputs, for example, proton addition. Due to the perspective of using protonated forms [1] in the design of molecular devices, for instance, Sps can be used as components for proton transfer in photoelectric cells, we focused on the effect of protonation on the isomerization pathway. The highest barrier (around 37 kcal/mol) on the reaction pathway corresponds to the proton transfer from N to pyran O. Thus, in this work we are looking for possible environments for decreasing the energy barrier during proton transfer from N to O atom in SP molecule and acceleration the protonated spiropyran-merocyanine (MC) transformation. One of such conditions are localization water molecule between N and O atoms and the effect of the external field.

Water molecule contributes to proton transfer from N to O atom. It has high conductivity, so protons move very quickly in this environment. Proton of the SP molecule joins to the water molecule and causes water molecule to lose its proton which attaches to the pyran O. This attachment leads to the elongation of the Cspiro-O bond with subsequent conversion from SP to MC. At the same time the energy barrier decreases on 6 kcal/mol. The external field with strength of 0.02 and 0.03 a.u applied towards pyran O direction can significantly reduce the energy barrier corresponding for proton transfer. As well, field effect can stabilize the SP molecule protonated on N atom.

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## **Instrumented nanoindentation as a method for mapping of properties of multi-phase Gd-doped ferromagnetic shape memory alloy**

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In a group of modern smart materials NiMnGa-based ferromagnetic shape memory alloys (FSMA) emerge as very promising materials due to their unique multifunctional behaviour, such as magnetic shape memory effect (MSME), superelasticity, magnetocaloric effect (MCE) or giant magnetoresistance (MR) [1].

Mechanical properties of FSMA are crucial when it comes to their potential applications as sensors, actuators or components of MEMS devices. Whereas the size and scale of investigated alloys are very small, standard methods for mechanical properties testing appear to be insufficient. Considering that, instrumented nanoindentation technique seems to be one of the complementary solution for investigations of hardness and elastic modulus. Constant and precise acquisition of load and displacement of the indenter tip during the indentation allows to determine these properties with a high accuracy. As a result, both plastic and elastic mechanical properties of investigated material may be examined [2].

In this research a series of nanoindentation tests were carried out on multi-phase Gd-doped  $\text{Ni}_{50}\text{Mn}_{25}\text{Ga}_{20}\text{Gd}_5$  ferromagnetic shape memory alloy. The Oliver-Pharr method were utilized to analyze recorded measurements [3]. Then nanoindentation tests results were used to map the mechanical parameters on the sample's surface. Obtained results were also correlated with multi-phase microstructure of alloy. The research was additionally supplemented by Atomic Force Microscope (AFM) measurements performed in contact mode (C-AFM).

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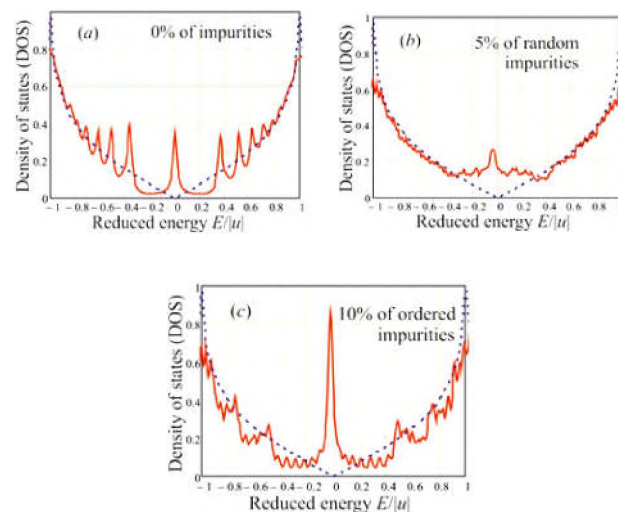
### Influenced electronic states in doped graphene: external magnetic field vs. impurity configurations

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We study magnetoelectronic structure of impure graphene applying the Peierls tight-binding model. To calculate electron density of states (DOS), we implement numerical algorithm using Green's functions, continued fraction technique and tridiagonalization for Hamiltonian. A perpendicular magnetic field  $B$  results in discrete Landau energy levels broadening as field  $B$  increases (Fig. 1a). Disordered and small content of ordered impurities smear and suppress Landau levels except the peak at a zero energy  $E$  (Fig. 1b). However, Landau levels re-appear on DOS curves for high concentrations of ordered impurities (Fig. 1c).



**Fig. 1.** Numerically calculated densities of electronic states (in units of hopping integral  $u$ ) for pristine (a) and impure (b, c) graphene sheets in a perpendicular magnetic field ( $B = 1000$  T), where 5 % (b) and 10 % (c) of impurity atoms are distributed randomly, i. e. disorderly, (b) or orderly (c). Dashed curves are obtained from analytical expression [1] for pristine graphene without magnetic field

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## Nanostructural clustering in the bulk magnetoresistance

### $\text{La}_{0.6}\text{Sr}_{0.15}\text{Bi}_{0.15}\text{Mn}_{1.1-x}\text{Ni}_x\text{O}_{3-\delta}$ ceramics

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According to X-ray diffraction data, the obtained ceramics  $\text{La}_{0.6}\text{Sr}_{0.15}\text{Bi}_{0.15}\text{Mn}_{1.1-x}\text{Ni}_x\text{O}_{3-\delta}$  with  $x = 0; 0.05; 0.1; 0.15; 0.2$  and  $0.3$  were single-phase with a rhombohedral  $R\bar{3}c$  type of distortion. The lattice parameter of a perovskite structure slightly changed with increase in  $x$ . On the basis of the defect formation mechanism [1] with using iodometric titration method and thermogravimetric analysis, it has been established that the real structure is a defect and contains variable valence manganese  $\text{Mn}_A^{2+}$ ,  $\text{Mn}_B^{3+}$  and  $\text{Mn}_B^{4+}$  ions as well as cationic  $V^{(c)}$  and anionic  $V^{(a)}$  vacancies. The presence of vacancies leads to the appearance of superstoichiometric manganese  $\text{Mn}_A^{2+}$  ions in  $A$ -positions of the perovskite structure with a formation of nanoscale planar clusters of  $\sim 10\text{--}25$  nm [2, 3]. A planar character of the  $\text{Mn}_B^{4+} - V^{(a)} - \text{Mn}_A^{2+} - \text{O}^{2-} - \text{Mn}_B^{4+} - \text{O}^{2-} - \text{Mn}_B^{3+}$  clusters results of the interruption of exchange interactions by  $V^{(a)}$  vacancies. The conclusion about the presence of the nanostructural planar clustering is confirmed by the results of magnetic measurements at  $T = 77$  K. In the compositions with  $x = 0.05$  and  $0.1$ , the anomalous magnetic hysteresis is due to  $90^\circ$  exchange antiferromagnetic interactions ( $\text{Mn}_A^{2+} - \text{O}^{2-} - \text{Mn}_B^{(3,4)+}$ ) between the nanostructural cluster and the ferromagnetic matrix structure.

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### **XRD investigation of structural transformations in InSb induced by ion implantation**

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Strain profiles for the damaged layers were reconstructed from the diffraction curves obtained by the high-resolution X-ray diffraction (HRXRD) using X'Pert PRO MRD diffractometer. The distribution of intensity in the vicinity of the InSb(111) and (333) reciprocal lattice point was analysed using a triple-axis arrangement. To reconstruct the profiles an autofitting procedure, based on a genetic algorithm [1, 2], was used. X-ray reflectometry method was used to get an electron density depth profiles in the damaged layers. It was found that the shape of the strain profiles depends on a chemical activity of the impurity. It can be a result of a quasi-chemical interaction between radiation-induced defects and impurity atoms. Density profiles obtained from XRR data for the thin (3–4 nm) surface layer are different for a one- and two-step implantation process. For all types of the implanted ions, the second step increases the surface layer roughness.

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**ROS-sensitive luminescence of  $\text{Ce}^{3+}$  ions in nanoceria  
allowing visualization of its antioxidant action  
by spectroscopic techniques**

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Nanocrystals of cerium dioxide (nanoceria) due to their unique ability to regeneration of antioxidant properties present nowadays one of the most perspective classes of redox-active materials for treatment of the negative consequences of an oxidative stress determined by action of reactive oxygen species (ROS) in a living cell. In our investigation we show that nanoceria beyond being effective ROS scavenger can act also as the ROS sensor allowing to determine ROS concentration in the cell. Moreover, using specific luminescent properties of nanoceria determined in our research, antioxidant characteristics of nanoceria can be easily controlled and its action in biological substances can be visualized by conventional spectroscopic techniques.

Our investigations involving both of UV-vis and synchrotron radiation have shown that luminescence properties of nanoceria are determined by the presence and concentration of  $\text{Ce}^{3+}$  ions in nanoceria lattice. Content of  $\text{Ce}^{3+}$  ions is closely connected with concentration of oxygen vacancies and depends strongly on the size of nanocrystal, atmosphere of treatment and presence of doped ions with different valence ( $\text{Y}^{3+}$ ,  $\text{Eu}^{3+}$ ) or ionic radius ( $\text{Zr}^{4+}$ ,  $\text{Hf}^{4+}$ ). We have shown that at UV excitation intensive  $5d \rightarrow 4f$  luminescence band of  $\text{Ce}^{3+}$  ions is observed in nanoceria at 390 nm. Nature of this band was confirmed by its excitation spectra obtained using synchrotron radiation (HASYLAB, DESY, Hamburg) which shows distinct five-fold splitting typical for f-d transitions.

Content of  $\text{Ce}^{3+}$  ions in  $\text{CeO}_2$  determines also the antioxidant properties of this material, so intensity of  $\text{Ce}^{3+}$  luminescence can be used as a measure of antioxidant ability of ceria nanocrystals. Addition of hydrogen peroxide (the most widespread type of ROS) to nanoceria solution leads to fall of  $\text{Ce}^{3+}$  band intensity due to transfer of the part of  $\text{Ce}^{3+}$  ions to  $\text{Ce}^{4+}$  ones. The portion of  $\text{Ce}^{3+}$  ions underwent  $\text{Ce}^{3+} \rightarrow \text{Ce}^{4+}$  transition increased with increase of the concentration of the oxidant. So, using intensity of  $\text{Ce}^{3+}$  luminescence band as a measure, the antioxidant action of ceria can be easily controlled by conventional spectroscopic techniques. ROS scavenging properties of nanoceria along with absence of toxicity for nanoparticles with sizes in the range of 5–15 nm allow using nanoceria as an effective antioxidant material able both to detect and to regulate ROS concentration in living cells.

### **The investigation of the fundamental properties (Ga, Mn)As and (Ga, Fe)As LT-MBE nanolayers**

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We have investigated (Ga, Fe)As and (Ga, Mn)As nanolayers, grown by LT-MBE. The alloy compositions were determined using high resolution X-ray diffractometry (XRD) followed by the in-situ Reflection High Energy Electron Diffraction (RHEED). The SQUID magnetometry have been used for the study the epi-layers evolution from the diamagnetism to the soft ferromagnetism with the increasing of the doping level. Photorefectance (PR) measurements enabled the determination of the band gap ( $E_0$ ) optical transitions in (Ga,Mn)As and (Ga,Fe)As. PR studies were supported by  $\mu$ Raman spectroscopy and Angle Resolved Photoemission Spectroscopy (ARPES). We have observed the built-up of the Mn states on the GaAs valence band edge resulting in appearance of the additional below band gap optical transition for the n-type (Ga, Mn)As epitaxial layers. The n-type - p-type transition in (Ga, Mn)As is combined with the merging of the Mn acceptor sub-band and the (Ga, Mn)As valence band. The paramagnetic – ferromagnetic transition is combined with the small blue shift of (Ga, Mn)As gap. Our results obtained for the ferromagnetic (Ga, Mn)As can be well explained by the contribution of the band gap renormalization, increasing of the strain and disorder with the increasing of Mn concentration, as well as by two main electronic effects: the Moss-Burstein band filling effect (gap's blue shift) and the band gap narrowing (gap's red shift) which usually exist in degenerate p-type semiconductors. The (Ga, Fe)As epitaxial layers do not reach the ferromagnetic phase because the Fe ions are not acceptor impurities and do not modify the valence band of GaAs host.

**Effect of electric field and position of impurity  
on energy spectrum of electron and its location  
in multilayered quantum dot**

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Modern technology allows growing complicated spherical nanostructures which consist of core and several layers. At their base it is possible to create the white light sources, highly efficient fluorescent labels, detectors and solar elements.

The optical properties of multilayered quantum dots depend both on materials compositions and layers sizes, on location of impurities [1–2] and the effect of external fields [3] too.

In the paper we study the electron energy spectrum and wave functions in CdSe/ZnS/CdS quantum dot, driven by uniform electric field with and without interaction with off-central donor impurity (ion). The polarization effects appearing due to the different values of dielectric constants of neighbor layers are taken into account in numerical calculations.

It is shown that under the effect of electric field the electron changes its location from core into the outer layer of nanoheterostructure. The binding energy of electron with impurity depends both on the location of impurity and intensity of electric field. The change of quasi-particle location influences on the energies and intensities of intraband quantum transitions.

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## **Ferromagnetism and band structure engineering in the (Ga, Mn)As, Ga(Bi, As) and (Ga, Mn)(Bi,As) nanolayers**

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The GaAs based ferromagnetic semiconductor alloy compounds containing Mn and Bi emerged as potential candidates for novel nanoelectronic and spintronic application. The (Ga,Mn)As, Ga(Bi,As) and (Ga,Mn)(Bi,As) nanolayers are grown using low temperature (230 °C) molecular beam epitaxy (MBE). The alloy compositions are determined with high resolution X-ray diffractometry (XRD) followed by the in-situ Reflection High Energy Electron Diffraction (RHEED). The superconducting quantum interference device (SQUID) magnetometry is used for the investigation of the magnetic properties of the heterostructures.

Photoreflectance (PR) measurements are used for the determination of the band gap (E<sub>0</sub>) and spin-orbit split-off (ESO) band to conduction band optical transitions. Besides the PR technique, the samples have been investigated by the  $\mu$ Raman spectroscopy to confirm p-type character of some films by the observation of the Coupled Plasmon-LO Phonon Mode (CPPM). The in-situ UV Angle Resolved Photoemission Spectroscopy (ARPES) is used for the band structure analysis of the epitaxial layers. The low temperature optical-energy-gap measurements supported by complementary characterization, for a series of (Ga,Mn)As, Ga(Bi,As) and (Ga,Mn)(Bi,As) nanolayers, show that the deep modification of the GaAs valence band caused by Mn incorporation occurs for a Mn content much lower than that supporting dilute ferromagnetic phase in the investigated nanofilms.

# **Session 6**

## **Nanostructured Surfaces**

**Dislocation-assisted phase separation processes  
in binary systems subjected to irradiation**

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We extended the model of phase separation with a dislocation mechanism in binary systems subjected to irradiation taking into consideration stochastic conditions. And have studied the role of the fluctuation effects in the prototype model of binary systems undergoing phase separation assisted by mobile dislocations. We considered spatial correlations of these fluctuations and the effect of spatial correlations onto phase decomposition processes.

Irradiation is described by athermal atomic mixing in the form of ballistic flux with spatially correlated stochastic contribution. While studying the dynamics of domain size growth we have shown that the dislocation mechanism of phase decomposition delays the ordering processes. It is found that spatial correlations of the ballistic flux noise cause segregation of dislocation cores in the vicinity of interfaces effectively decreasing the interface width. A competition between regular and stochastic components of the ballistic flux is discussed.

**Investigation of  $\text{XO}_4^{2-}$  ( $\text{X} = \text{Cr, Mo, W}$ ) molecular oxyanions adsorption on surface of carbon nanostructures in aqueous solution**

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Carbon nanotubes (CNTs), as one of the representative nanostructured carbon materials, continue to attract attention in the past two decades due to their unique physical and chemical properties. In particular, chemical functionalization of CNTs can modify their physical and chemical properties, leading to the improvement of their performance for specific applications. Notably, some studies have indicated that functionalized CNTs are a promising candidate for the removal of toxic heavy metals from waste water. Theoretical modeling of molecular adsorption on the surface of CNTs can provide a quantitative description of adsorption capacities of CNT-based materials.

In this work we considered adsorption characteristics of the  $\text{XO}_4^{2-}$  ( $\text{X} = \text{Cr, Mo, W}$ ) molecular oxyanions on the surfaces of pure and N/B-doped CNTs and graphene sheets. DFT-based geometry-optimized calculations of the electronic structures of carbon nanostructures with adsorbed oxyanions were carried out by Gaussian 09 program package [1]. Binding energies between oxyanions and adsorbents, relaxed geometries, electronic wavefunction contours were calculated and analyzed. Effects of water solvent on studied adsorption case are considered with the polarisable continuum model (PCM).

Obtained results were discussed in view of potential application of the CNT-based materials as efficient adsorbents of toxic hexavalent metals oxides.

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## **The effect of the modification of sol-gel silica coatings on the anticorrosion properties on metallic substrates**

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Metallic materials are one of the most widely used construction material. They often work in aggressive environments (hot gases, chlorides etc.) which are a reason of degradation processes (such as corrosion and erosion). These degradation processes, mainly corrosion, causes huge economic losses. According to the National Association of Corrosion Engineers (NACE), the global costs of corrosion are about 3.4 % of the gross national product (GNP) of USA [1]. On the other hand, many number of regulations (eg. Directive of UE 2000/53/EG) limit the possibility of using hexavalent chromium, which is used in the most effective method of protection against corrosion [2].

Currently, the sol-gel technique is a rapidly developing method of obtaining environmental friendly materials [3]. Sol-gel materials can be an alternative to hexavalent chrome compounds [2]. In additional, this is a method which enables production of materials with different molecular-controlled properties and wide spectrum of their use [4].

The present paper shows changes of electrochemical properties of 316L substrate, coated by sol-gel coatings. The experiment was conducted under the 3 % NaCl environment. Results indicate significant improvement in corrosion resistance of 316L stainless steel after hybrid SiO<sub>2</sub>/ZrO<sub>2</sub>/GPTMS coated.

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### **SPV decays of silicon structures with composite epoxy – polymer films**

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Surface photovoltaic (SPV) presentation the process what answering about accompany photogeneration [1].

In this work, we study the temporal behavior of the photoinduced charges decay in composite epoxy – polymers film deposited on silicon surface. We used sandwich cell with giga ohm amplifier for detect SPV signal. The sandwich cell is experimental setup what works for the capacitor what contains sample charged from photoinduced charge.

The object of study selected industrial epoxy oligomer ED-20 mark, which have highly adhesive and cohesive strength, as a filler nano particles SiO<sub>2</sub>. As substrate used to prototypes served a standard monocrystalline silicon wafer (c-Si) with orientation (100).

SPV, sensitive, in particular, to State of the interface through the effects of surface and interface recombination, scattering into lattice and on chaotically distributed defects.

Molecular junctions would enable utilizing the incredibly diverse range of chemistries that currently exist to expand the electrical properties of inorganic solid state devices [2].

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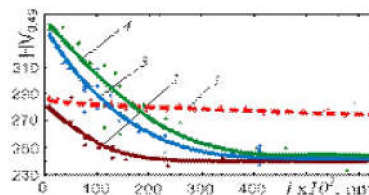
# **The influence of vacuum treatment of different range on size hardened subsurface layers of the HFE-1 hafnium alloy**

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High affinity Hafnium to oxygen influences on the functional properties of products [1–2]. Results influence composition of medium annealing on properties plates (~ 1 mm) HFE-1 hafnium alloy it was showed. It was found that annealing ( $T = 850\text{ }^{\circ}\text{C}$ ,  $\tau = 2\text{ h}$ ) in oxygen-containing atmosphere at  $P = 1.33 \times 10^{-2}\text{ Pa}$  is accompanied by the formation of a diffusion hardened subsurface layers of 30 000 to 35 000 nm with the  $\Delta\text{HV} = 100$  hardness gradient (Fig. 1).



**Fig. 1.** The distribution of micro hardness over the cross-section of hafnium specimens after treatments ( $T = 850^{\circ}\text{C}$ ,  $\tau = 2\text{ h}$ ) in depending on the vacuum: 1 – initial state; 2 –  $P = 1,33 \cdot 10^{-3}\text{ Pa}$ ; 3 –  $P = 1,33 \cdot 10^{-2}\text{ Pa}$ ; 4 –  $P = 1,33 \cdot 10^{-1}\text{ Pa}$

Was found that the hardness gradient in the surface of the metal layer of the samples after the treatment decreases monotonously from the surface to the middle of the sample, indicating the absence of dense phase films. The metal core hardness is decreased relative to the original state because of relaxation of residual stresses from rolling. As expected the highest hardness gradient is observed for the highest vacuum.

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### Structure and morphology study of carbon nitride nanostructured films under nanosecond laser pulses

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The enhanced study of carbon nitride nanostructured films  $CN_x$  are motivated by a theoretical prediction of the  $C_3N_4$  phase with physical characteristics exceeding diamond [1, 2]. Pulsed laser annealing of carbon films can significantly change their structure, surface morphology and electrophysical properties [3].

Laser annealing of  $CN_x$  films was carried out in a pulsed mode ( $t_p = 10$  ns,  $\lambda = 535$  nm) of a YAG:  $Nd^{3+}$  laser. The structure and surface morphology of films was studied by Raman spectroscopy and atomic force microscopy (AFM).

The surface morphology of the initial  $CN_x$  films is represented by nano-needles formation, whose height increases with increasing laser radiation intensity. The two-peak structure with features of D and G bands near  $1385$  and  $1580\text{ cm}^{-1}$  which has been observed by the Raman spectra demonstrates some reduce of the relation of bands heights with increase of laser intensity. The high intensity of the D mode  $1385\text{ cm}^{-1}$  indicates the presence of defectiveness of the nanocolumns structure after laser irradiation, which is associated with the defects increasing of the nanocolumns structure due to possible not congruent erosion. The possible mechanisms of this processes are discussed.

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## **XPS and AFM studies of impact of the surface oxidation on the properties of $\text{Bi}_2\text{Te}_3$ thin films**

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Topological Insulators (TI), a novel class of quantum materials [1] are considered as promising materials for multiple applications in next generation electronic or spintronic devices. The existence of metallic surface states on insulating bulk is the most important feature of this class of materials. However it is well known that defects, strains and doping influence that important feature of the TI's. In our studies we focused on impact of surface oxidation on properties of one of known TI's –  $\text{Bi}_2\text{Te}_3$ .

We used X-ray photoelectron spectroscopy (XPS) and atomic force microscopy (AFM) to study behavior of  $\text{Bi}_2\text{Te}_3$  films of different thicknesses exposed to the atmosphere. With the use of MBE system we have grown step-like sample with thicknesses of particular  $\text{Bi}_2\text{Te}_3$  layers ranging from 40 to 100 Å. The sample was grown on mica substrate in the co-deposition mode as described in our previous work [2]. The electron diffraction measurements (RHEED) confirmed monocrystalline structure of the film. The studies of electronic structure, focused on the analysis of the Bi4f, Te3d and O1s core levels, were realized after the deposition and after the oxidation process. The results indicate formation of  $\text{Bi}_2\text{Te}_3$  compound, and further, after exposition to the air the oxidation of the film surface. The AFM measurements realized after oxidation process revealed grainy structure of deposited films and thickness dependent changes of the surface roughness ranging from 0.3 to 2.25 nm. Additional features as presence on selected films of fusiform grains, channels and craters were detected.

*This work was supported by Research Grant NCN 2016/21/B/ST5/02531.*

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# **Session 7**

## **Physico-Chemical Nanomaterials Science**

## Corrosion inhibition efficiency of green synthesised silver nano particles in acidic medium

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Nanostructured materials (1–100 nm) have attracted tremendous interest as corrosion inhibitor due to their high surface area on the metal surfaces. Nanotechnology is concerned with the development of experimental processes for the synthesis of nanoparticles of different sizes, shapes and controlled disparity [1]. The synthesis of nanoparticles by chemical and physical method is very expensive[1]. In this study, the green synthesis of silver nanoparticles (AgNPs) was carried out by *Nicotiana tabacum* leaves extract as reducing agent and characterized using UV-Vis, FT-IR spectrophotometer, X-ray diffraction and SEM analysis[2]. The corrosion inhibition efficiency of the *Nicotiana tabacum* leaves extract[3] and synthesized AgNPs (nano-green inhibitor) on mild steel in acidic solution was determined by Gravimetric method. The results suggested that nanogreen inhibitor (AgNPs) is more effective than green inhibitor (leaves extract). Furthermore, with the increasing concentration, %IE increases for both types of the inhibitors. The Scanning Electron Microscopy (SEM) techniques were performed for examine surface morphology of metal (specimen) in absence and presence of both inhibitors. The outcomes indicated a formation of a protective layer over metal (specimen) which prohibited the corrosion phenomena. The experimental results obtained show that the Ag nanoparticle from *Nicotiana tabacum* leaves extract is an excellent eco-friendly corrosion inhibitor for mild steel.

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**Stabilization of magnetite nanoparticles by sodium citrate****Pesina D. A., Bereznyak E. G., Dukhopelnikov E. V., Gladkovskaya N. A.**

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Targeted drug delivery using magnetic field is one of the promising trends of the use of magnetic nanoparticles (MNP), magnetite  $\text{Fe}_3\text{O}_4$  nanoparticles in particular. Modification of their surface which allows to ensure the stability of their aqueous colloidal solutions and to create stable complexes with drugs is a necessary requirement for biomedical use of MNP [1]. Trisodium citrate (NaCit) is one of the widely used biocompatible MNP stabilizers. Nevertheless, there is no consensus on its optimal concentration required to stabilize MNP.

In the present work, the coagulation stability of colloidal MNP solutions as a function of NaCit concentration ( $C_{\text{NaCit}}$ ) was studied using spectrophotometry.

The MNP sample was placed in solutions of sodium citrate with  $C_{\text{NaCit}} = 10^{-5} \div 10^{-2} \text{ M}^{-1}$ . Then two modes of ultrasound dispersion were applied: 22 kHz for 10 min and 44 kHz for 120 min. Absorption spectra were recorded in the 330–600 nm range immediately after ultrasound processing and 72 hours later. The concentration of MNP ( $C_{\text{MNP}}$ ) was determined from the absorption value at the maximum of the band at 340 nm.

Analysis of the spectra showed that dispersion at 44 kHz allowed us to obtain colloidal solutions with a higher concentration of MNP and more stable in time. After application of this mode of ultrasound dispersion, 80 % of the MNP remained in the solution after 72 hours.

Dependences of  $C_{\text{MNP}}$  in solution on  $C_{\text{NaCit}}$  showed that the decrease in MNP coagulation was observed for  $C_{\text{NaCit}}/C_{\text{MNP}}$  ratios up to  $(1.3\text{--}1.6) \cdot 10^{-2} \text{ mol/g}$ . The further addition of NaCit does not lead to any changes of the amount of MNP in the solution.

Sedimentation curves allowed us to plot the differential distribution curve and estimate the average diameter of the MNP in the dispersion systems under consideration. Addition of NaCit leads to a decrease of MNP aggregation.

For all  $C_{\text{NaCit}}$  studied, application of magnetic field results in a complete coagulation of MNP from the solution. This indicates that their magnetic properties are preserved.

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## BEA zeolite design for lactic acid dehydration

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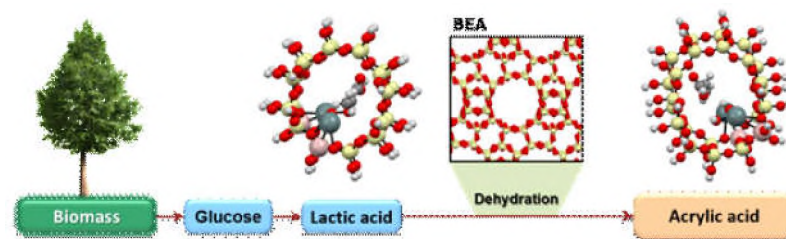
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The main goal of our studies is design of zeolite catalyst for the production of acrylic acid from biomass derived lactic acid. The theoretical modeling of lactic acid dehydration helps in further development and synthesis of zeolite with declare structure and obtaining structure of substrates, products and intermediates.

The electronic structure of all clusters has been calculated by *ab initio* density functional theory (DFT) methods (program StoBe) using the non-local generalized gradient corrected functionals according to Perdew, Burke, and Ernzerhof (RPBE), in order to account for electron exchange and correlation. A  $\text{Al}_2\text{Si}_{22}\text{O}_{64}\text{H}_{32}$  cluster was chosen to represent part of a single pore in the BEA zeolite. The stabilization of monomeric and dimeric metal complexes, such as M-OH, HO-M-O-M-OH and M-O-M, in the BEA pore has been investigated (where M = Fe, Sn, V, Cu).

Possible modes of interaction of lactic acid with different cations (Si, Al, Fe, Sn, V, Cu) in BEA zeolite framework as well as with added metal nanoparticles have been considered. The interactions of lactic acid is observed only above M-O-M dimmer. The hydrogen abstraction from methyl group over different oxygen and OH interactions with metallic sites of dimmer in the zeolite framework have been observed, which succeed in acrylic acid formation (Fig. 1).



**Fig. 1.** Scheme illustrating the lactic acid dehydration inside BEA zeolite

*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. 665778. (Polonez-1 2015/19/P/ST4/02482).

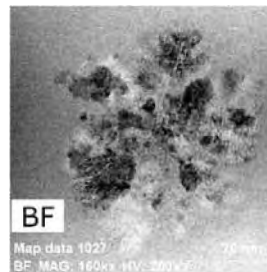
## Effect of Ga on the nanostructure of As-Se-based glasses

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Se-based chalcogenide glasses (ChG) have found widespread application in modern chalcogenide photonics because of their superior transmittance in IR spectral region up to 20–25  $\mu\text{m}$ . This functionality can be further stretched by doping ChG with some rare-earth (RE) activators like  $\text{Pr}^{3+}$ ,  $\text{Tb}^{3+}$ ,  $\text{Er}^{3+}$ , etc., which possess numerous radiative transitions emitting in near and mid-IR range up to 10  $\mu\text{m}$  thus providing advanced optical active fibers. To be functioning, the RE atoms should occupy an electrically active “+3” state, which is principally impossible for typical ChG under a condition of global electroneutrality proper to full saturation of covalent bonding. Local structural nanoinhomogeneities possessing an effective negative electrical charge are crucially desirable to compensate positive electrical charge of RE ions embedded in covalent-linked glassy skeleton. This problem can be resolved extrinsically due to some chemical modifiers such as Ga or In added to ChG in small amounts, which don't disturb their glass-forming ability.



**Fig. 1.** Microstructure cut-section of  $\text{Ga}_4(\text{As}_{0.40}\text{Se}_{0.60})_{96}$  in STEM bright field

In this report, the nanostructure of RE-doped As-Se-based glasses modified by Ga was studied using transmission electron microscopy with EDS analyzer, positron annihilation lifetime spectroscopy, etc. It was shown that Ga additions into the ChG matrix provokes crystallization of  $\text{Ga}_2\text{Se}_3$  phase as it was identified by transmission electron microscope (Fig. 1). The finalizing nanostructurization due to RE-doping is explained in terms of two-state positron trapping model.

## **Influence of cobalt doping on structural and optical properties of co-precipitated $\text{ZnFe}_2\text{O}_4$**

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Spinel ferrite nanomaterials (SFNMs) with general molecular formula  $\text{MFe}_2\text{O}_4$  (where  $\text{M} = \text{Mn, Fe, Co, Ni, Cu, Zn}$ ) have gained huge attention nowadays from fundamental science point of view owing to their unique properties and promising numerous applications such as high-density data storage, catalysts, gas sensors, rechargeable lithium batteries, information storage systems, magnetic bulk cores, magnetic fluids, microwave absorbers and medical diagnostics and therapy, etc. The fundamental understanding of crystal chemistry in SFNMs is very essential and the proper choice of synthesis route will determine its crystal lattice structure and chemical composition, leading to enhanced/excellent physical and chemical properties. The aim of this study is to investigate in-depth the effect of  $\text{Co}^{2+}$  ions doping on  $\text{ZnFe}_2\text{O}_4$  nanoparticles in terms of crystal structure, morphology, magnetic and optical properties.  $\text{Zn}_{1-x}\text{Co}_x\text{Fe}_2\text{O}_4$  ( $x = 0.0; 0.1; 0.2; 0.3; 0.4; 0.5$ ) powders were prepared by co-precipitation method. X-ray diffraction and energy dispersive spectroscopy confirmed the involvement of  $\text{Co}^{2+}$  ions in  $\text{ZnFe}_2\text{O}_4$  lattice, an increase of the crystallite size from 37 to 51 nm in agreement with TEM analysis. FTIR revealed a slight change in two main bands  $\nu_1$  and  $\nu_2$  in the frequency range of  $400\text{--}4000\text{ cm}^{-1}$ , which caused by stretching vibrations at the A- and B-sites respectively. The elastic moduli such as stiffness constant, Young's modulus, rigidity modulus, bulk modulus, Poisson's ratio, wave velocity and the Debye temperature have been calculated using FTIR data. VSM showed transformation of magnetic behavior from paramagnetic to ferromagnetic as a result of  $\text{Co}^{2+}$  ions doping. With higher  $\text{Co}^{2+}$  ( $x = 0.2$  to  $x = 0.5$ ) content, the saturation magnetization (Ms) increased rapidly from 5.7 emu/g to 82 emu/g respectively. The remanence magnetization (Mr) and coercivity (Hc) were influenced by  $\text{Co}^{2+}$  content too and this was mainly related to the change in crystallite size. The optical band gap (Eg) of Co-Zn ferrites determined by means of diffuse reflectance spectra (Tauc plots) was found to decrease with  $\text{Co}^{2+}$  content, setting in the range 1.89–1.31 eV.

## Micro-/nano-structured materials for H<sub>2</sub> energy

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Renewable, clean and sustainable energies are of great importance for the modern society. Extensive research, funding and policies are devoted toward the development and implementation of such energies. Hydrogen has been identified as a very promising energy carrier, as it can be stored as gas, liquid and solid namely metal hydrides.

Both structural (phase transformation, substitution, interstitial, doping) microstructural (composites, particles/grains size reduction, defects, imperfections) modifications introduce important changes into material's properties.

Furthermore, materials at the nanoscale offer diverse tuneable properties as a function of their shape/size due to high surface area and quantum confinement. Thereby, nanostructured materials exhibit enhanced properties compared to bulk counterparts in terms of high-density reversible H<sub>2</sub>, faster kinetics, reduced desorption/absorption temperature and better cycling.

In this paper, selected micro- and nano-/structured materials will be presented including mainly: (i) composites where the kinetic can be improved by the precipitation of secondary phase; (ii) MgH<sub>2</sub>/based nanocomposites; (iii) effect of catalysts (Fe<sub>2</sub>O<sub>3</sub> and NiO) on the formation of carbon nanostructures and their H<sub>2</sub> properties and (iv) Lithium reactivity with metal hydrides (i.e. NiTi) for a new generation of Li-MH rechargeable batteries. Density functional theory (DFT) calculations will be presented to discuss the electronic structure, enthalpy for the stability of alloys/hydrides, etc.



### **Influence of pressure changes during sulfurization on formation of thin film $\text{Cu}_2\text{ZnSnS}_4$ solar cell absorber**

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$\text{Cu}_2\text{ZnSnS}_4$  (CZTS) is a promising light absorber material for the production of thin film (TF) solar cells due to its desirable direct optical gap of 1.5 eV and large band-to-band optical absorption coefficient ( $\sim 10^5 \text{ cm}^{-1}$ ). All constituents of CZTS used to utilized in processing are non-toxic and abundant in the earth crust with contrast to well studied CdTe and  $\text{Cu}_2\text{In}(\text{Ga})\text{S}(\text{Se})_2$  absorbers. The conversion efficiency record of CZTS-based TF SCs reaches value of 12.6 % [1] that it is not enough for industrial production. The aim of this work was to investigate the structure properties of CZTS TF grown by a two-step synthesis at different pressure in vacuum chamber.

Obtained samples were measured by Energy-Dispersive X-ray spectroscopy (EDX) equipped inside a scanning electron microscope (SEM). All samples are Cu-poor and Zn-rich, the deviation of stoichiometry by S and Sn is immaterial. The structural properties of the CZTS were explored using the  $\mu$ -Raman spectroscopy in backscattering configuration. From the Raman spectra we estimated the degree of the kesterite structure disordering. The phases forming during processes were studied using X-ray diffraction (XRD) spectroscopy. On the XRD-spectra of all samples present weak peak at  $29^\circ$  that confirms the presence of a small amount  $\text{Cu}_2\text{S}$  and  $\text{CuS}$  in the structure of CZTS thin films. We can resume that the most stoichiometric sample was created by sulfurization at pressure of argon 450 mbar. It was evidenced by the presence of the most intense peaks characteristic of CZTS. The influence of pressure in vacuum chamber on the CZTS thin films formation was investigated. Raman-spectra suggests that the high pressure facilitate to create more ideal kesterite structure.

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## Obtaining and studying $\text{NaNd}_9(\text{SiO}_4)_6\text{O}_2$

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Compounds with apatite structure are used as biomaterials, luminescent substances and laser materials [1, 2], matrices for the absorption of actinides, solid electrolytes for fuel cells – environmentally friendly sources of electricity [3, 4].

The double silicate  $\text{NaNd}_9(\text{SiO}_4)_6\text{O}_2$  with apatite structure was synthesized by ceramic methods. It was studied by the method of rhengen phase analysis (XRD), the refinement of the crystal structure was carried out by the Rietveld method. The resulting compound was also studied by scanning electron microscopy (SEM).

The synthesis was carried out at a temperature of 800 and 1100°C for 120 hours. The chosen synthesis technique prevented the sublimation of sodium oxide.

Under these conditions of synthesis, homogenization of the samples is achieved due to the diffusion of the components. According to electron microscopy, the elements are practically uniformly distributed over the surface of the particle, which indicates the formation of a homogeneous sample. On the X-ray of the sample calcined under the conditions indicated above, only reflections from the structure of apatite are present.

Rietveld method established that the sodium atoms in the structure are arranged in an orderly fashion (in position 4f). O (4) oxygen atoms that are not part of the ion silicate are located in the centers of the triangles of Nd (2). The presence of sufficiently large distances Nd-Nd (3.940 Å) indicates the possibility of the existence of luminescent properties.

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## **The structural diagram of carbon-nitride films produced by reactive magnetron sputtering**

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Carbon structures with the nitrogen addition carbon-nitride CN<sub>x</sub> ( $x < 1$ ) films – have even more interesting and diverse properties than carbon films. A wide variety of structural modifications in depending on synthesis conditions explains the long list of potential applications of the carbon-nitride films. The novel technology of non-catalytic production of nanostructured carbon-nitride films [1] by magnetron sputtering of a graphite target have been proposed. The ranges of the external parameters that control formation of microstructure CN<sub>x</sub> films were determined.

A series of carbon-nitride CN<sub>x</sub> ( $x < 1$ ) nanostructured samples has been synthesized by reactive magnetron sputtering of a graphite target in the argon and nitrogen atmosphere in the conditions of low-temperature magnetron plasma. Magnetron plasma parameters (power, cathode current, pressure, a concentration of the plasma components, substrate temperature, distance from the substrate to the cathode, and others) was varying. Scanning electron microscopy and optical spectroscopy were used for structure characterization of the obtained CN<sub>x</sub> films. It gave a possibility to control the parameters of obtained nanocolumnar and fullerene-like structures in dependence on the substrate temperature and the concentration of nitrogen. The characteristic absorption bands were found by optical spectroscopy for the basic nanostructures of carbon-nitride CN<sub>x</sub> films. The structural diagram for the CN<sub>x</sub> films in depending on the substrate temperature and the concentration of nitrogen was built. It includes four allotropic CN<sub>x</sub> structures (graphite-like, fullerene-like, diamond-like and nanocolumnar structure) and mixed areas.

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## Thermodynamic properties of II-VI and IV-VI chalcogenide crystals in the cubic phase

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Cadmium and lead chalcogenide compounds are perspective materials for production on its base a number of highly efficient devices of nuclear power, solar technology, optical and acoustic electronics, X- and gamma-ray detectors, substrates for epitaxial growth, thermoelectric energy converters, electronic devices and others [1, 2]. The effective using of this materials both in model studies and practical applications caused by set of unique properties of lead telluride, in particular, because the small band gap, high carrier mobility and high dielectric constant.

Rock salt structure was selected for modeling studies because lead chalcogenides crystallize in the face-centered cubic lattice NaCl (structural type B1). These atom locations can be explained by the fact that lead chalcogenides belonging to polar semiconductors, characterized by ion-covalent type of bond. Cadmium chalcogenides usually crystallizes in the sphalerite structure, where each atom A (B) is located in the center of a regular tetrahedron, the 4 tops of which are the atoms of another element B (A).

Geometric and thermodynamic parameters of cubic CdX and PbX (X = S, Se, Te) crystals were obtained using the computer calculations of the thermodynamic parameters within density functional theory method DFT. Cluster models for the calculation based on the analysis of the crystal and electronic structure. Temperature dependence of energy  $\Delta E$  and enthalpy  $\Delta H$ , Gibbs free energy  $\Delta G$ , entropy  $\Delta S$  were determined on the basis of ab initio calculations of the crystal structure of molecular clusters. Analytical expressions of temperature dependences of thermodynamic parameters which were approximated with quantum-chemical calculation points have been presented. Experimental results compared with theoretically calculated data.

1. W. Biernack, U. Scherz and Ch. Schrepel. Local vibrational modes and anharmonic forces of  $Mg_2$  and  $S_2$  in ZnTe and CdTe crystals // Physical Review B., 1997. – **56**, N 8. – P. 4592–4596.

2. Zhang Y., Ke X., Chen C., Yang J., Ken P. R. C. Thermodynamic properties of PbTe, PbSe, and PbS: First-principles study // Physical Review B, 2009. – **80**. – P. 024304.

## **Raman scattering from organic molecules deposited on the noble metal nanoparticles and graphene**

**Heinsalu S.<sup>1</sup>, Dolgov L.<sup>1</sup>, Kavelin V.<sup>2</sup>, Fesenko O.<sup>2</sup>,  
Pidhirnyi D.<sup>2</sup>, Dovbeshko G.<sup>2</sup>**

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46, Nauky Ave., Kyiv 03039, Ukraine.*

Examples of both plasmonic and electron transfer influences on the Raman signals from the organic molecules deposited on graphene [1] and nanosized noble metal nanoparticles [2] are investigated in this work. Particularly graphene enhanced Raman scattering is detected for the adenine layer and compared with the SERS signal from adenine deposited on the surface previously decorated by noble metal nanoparticles.

Surface enhanced Raman detection and assignment of spectral bands for adenine as for a DNA constituent can be potentially important for those biomedical applications, in which monitoring of molecular conformations in DNA and its constituents is essential.

*This work was supported by NATO SPS project NUKR.SFPP 984702 and partially by the Estonian Research Council (institutional project IUT34-27), Marie Curie ILSES project no. 612620.*

1. Xu W., Mao N., Zhang J. Graphene: a platform for surface-enhanced Raman spectroscopy // *Small.*, 2013. – **9(8)**. – P. 1206–1224.
2. Schlücker S. Surface-enhanced Raman spectroscopy: concepts and chemical applications // *Angew. Chem. Int. Edit.*, 2014. – **53**. – P. 4756–4795.

**LECTURERS  
OF THE 4-th INTERNATIONAL  
SUMMER SCHOOL  
NANOTECHNOLOGY:  
FROM FUNDAMENTAL RESEARCH  
TO INNOVATIONS**



**Mohamed BOUODINA**

**QUALIFICATIONS AND EMPLOYMENT**

**Position:** Manger of Central Labs

**Professional affiliations:**

University of Bahrain

**Field of Your interests:** Nanotechnology,  
Materials Science, Energy

**PERSONAL INFORMATION**

**WORK EXPERIENCE:**

- 2010–2015: Director of the Nanotechnology Centre, University of Bahrain, Kingdom of Bahrain;
- 2006 – Present: Assistant Professor: Department of Physics, College of Science, University of Bahrain, Kingdom of Bahrain;
- 2005–2006: Assistant Professor: Department of Physics, College of Science, King Khalid University, Abha, Kingdom of Saudi Arabia;
- 2002–2005: Research Fellow: Department of Materials, School M3, University of Nottingham, UK;
- 1998–2002: Research Fellow, Department of Materials, Queen Mary University of London, UK;
- 1996–1998: Research Scientist, National Institute of Materials and Chemical Research, Tsukuba, Japan.

**EDUCATION AND TRAINING**

- Degree: Ph. D. (Honor) in Solid State Physics, University Joseph Fourier (UJF), Grenoble, France, 1995
- Achievements: Over 24 Invited/Plenary Talk, 260 Papers in ISI Journals; 2 Books (indexed by Scopus, IET, etc) and 20 Book Chapters; Editor (20) and regular Reviewer (35) for international journals, etc.

**Lecture title:** Micro-/Nano-Structured Materials for H<sub>2</sub> Energy.

**Lecture abstract:** Renewable, clean and sustainable energies are of great importance for the modern society. Extensive research, funding and policies are devoted toward the development and implementation of such energies. Hydrogen has been identified as a very promising energy carrier, as it can be stored as gas, liquid and solid namely metal hydrides.

Both structural (phase transformation, substitution, interstitial, doping) microstructural (composites, particles/grains size reduction, defects, imperfections) modifications introduce important changes into material's properties.

Furthermore, materials at the nanoscale offer diverse tuneable properties as a function of their shape/size due to high surface area and quantum confinement. Thereby, nanostructured materials exhibit enhanced properties compared to bulk counterparts in terms of high-density reversible H<sub>2</sub>, faster kinetics, reduced desorption/absorption temperature and better cycling.

In this paper, selected micro- and nano-/structured materials will be presented including mainly: (i) composites where the kinetic can be improved by the precipitation of secondary phase; (ii) MgH<sub>2</sub>/based nanocomposites; (iii) effect of catalysts (Fe<sub>2</sub>O<sub>3</sub> and NiO) on the formation of carbon nanostructures and their H<sub>2</sub> properties and (iv) Lithium reactivity with metal hydrides (i. e. NiTi) for a new generation of Li-MH rechargeable batteries. Density functional theory (DFT) calculations will be presented to discuss the electronic structure, enthalpy for the stability of alloys/hydrides, etc.



**Yuriy KHALAVKA****QUALIFICATIONS AND EMPLOYMENT****Position:** Ass. professor**Professional affiliations:** Department of Solid State Inorganic Chemistry and Nanomaterials of Yuriy Fedkovych Chernivtsi National University**Field of Your interests:** Nanochemistry, quantum dots, metal and semiconductor hybrid nanomaterials**PERSONAL INFORMATION****WORK EXPERIENCE:**

Since 2010 – Lecturer and researcher at Yuriy Fedkovych Chernivtsi National University.

2006–2007 – Scientist at the University of Mainz (Germany).

**EDUCATION AND TRAINING**

PhD in Solid State Chemistry – 2010.

2000–2005 – master of Chemistry, Yuriy Fedkovych Chernivtsi National University.

**Lecture title:** Tuning the quantum dots optical properties.**Lecture abstract:** Semiconductor quantum dots (QDs) with the emission in the near infrared region attract interest due to their potential applications as biomarkers for in vivo imaging, solar cells, telecommunication etc. For all of such applications it is important to control and to understand the effects of impurities on the band structure of nanoparticles.

On the other side blue-emitting quantum dots are desirable for down-conversion of the UV-light, sensing and lasing systems.

Doping of the nanoparticles is a versatile tool to extend optical properties for conventional materials. I will cover different aspects of nanoparticle doping and its influence on their luminescent properties.

The size dependence of the temperature coefficient (sensitivity) of the photoluminescence (PL) peak position of CdTe quantum dots will also be discussed. Temperature sensitivity increases as the average radius of CdTe quantum dots decreases. This must be taken into account in the design of solar light concentrators and light-emitting diode-monitors as well as other technologies in which a fine tuning of the light emission is important.

**Dr. Alessandro DAMIN****QUALIFICATIONS  
AND EMPLOYMENT****Position:** Research Technician**Professional affiliations:** University  
of Torino, Department of Chemistry**Field of Your interests:** Raman

spectroscopy, SERS substrates synthesis,  
study of catalytic systems through spectroscopic and computational  
methods.

**PERSONAL INFORMATION****WORK EXPERIENCE:**

Alessandro Damin is Research Technician and responsible for the maintenance and development of Raman Laboratory at Interdipartimental Centre NIS (Nanostructured Interfaces and Surfaces) of Università di Torino. He is involved in development of methodologies for Raman measurements of photo-sensible molecules (1 request patent deposited at Ministero dello Sviluppo Economico) and tools (e.g. controlled atmosphere and/or low-temperature cells) for the study of systems interesting in Chemistry Department and NIS Centre (e.g. carbon based functional materials, bio-glasses, materials interesting for cultural heritage and astro-chemistry, hydrides for H<sub>2</sub> storage). Furthermore he is responsible for the synthesis and/or characterization of innovative systems active in SERS (Surface Enhanced Raman Spectroscopy). He is also involved in the synthesis, development and characterization of model materials active in the catalysis of several processes (Cr doped glasses for the ethylene polymerization, Ti-doped glasses for the partial oxidation of alkenes, MoS<sub>2</sub> for de-sulphurization) and in photocatalysis (e. g. TiO<sub>2</sub> nano-particles embedded in high surface area glasses). Experimental data, mainly obtained through Raman, FTIR and UV-VIS spectroscopy both in reflectance and transmittance, are also interpreted through the adoption of ab-initio based modeling and the use of several dedicated code (Gaussian, NWchem, CRYSTAL).

**EDUCATION AND TRAINING**

– Chemistry Department (Università di Torino).

Thesis: “Ab initio based methods applied to the study of MgO and TS-1 case systems”. Tutor: Prof. ssa Silvia Bordiga.

– 1990–1998 – Degree in Industrial Chemistry at Facoltà di Scienze MFN (Università di Torino).

Thesis: “Study of oxidic systems by HRTEM and simulation techniques”. Tutor: Prof. G. Spoto.

**Lecture title:** Gold substrates for SERS: a material scientist point of view.

**Lecture abstract:** Abstract of the lecture SERS (Surface Enhanced Raman Spectroscopy) constitutes nowadays one of the most explored scientific subject, due to its potential application as a high sensitive technique, and with close connection to developments in the field of nanotechnology. In the present work, some of the results on several SERS active gold substrates (obtained in the Raman Lab at NIS Centre in Torino) will be reviewed, giving also some insights on problems occurring when very diluted species are investigated.

**Leonid YATSENKO**

**QUALIFICATIONS  
AND EMPLOYMENT**

**Position:** Director

**Professional affiliations:** Institute of Physics, the National Academy of Sciences of Ukraine.

**Field of Your interests:** Quantum optics, nanooptics, coherent excitation of atoms and molecules; mechanical action of laser light on atoms and molecules, metrology, laser physics.



**PERSONAL INFORMATION**

**WORK EXPERIENCE:**

Research fellow of the Institute of physics of NAS of Ukraine since 1979.

**EDUCATION AND TRAINING**

Master's degree (1976) – Moscow Physical Engineering Institute, Russia, Solid state physics.

Thesis: Nonlinear power resonances in ring gas lasers

Ph.D. (1980) – Lebedev Physical Institute, Moscow, Russia.

Thesis: The theoretical investigation of macroscopical parameters influence on the characteristics of optical frequency standards

Doctor of Science (1996) – Institute of Physics, Kyiv, Ukraine.

Thesis: Resonance phenomena in gas lasers.

**Lecture title:** Recent progress in optical trapping and manipulation of atomic, nano- and microobjects.

**Lecture abstract:** The history and recent advances in optical trapping and manipulation of atomic, nano- and micro objects will be presented. A brief introduction to physics of light momentum and history of light pressure will be followed by the general description of light forces on small objects. Special attention will be paid to laser cooling and trapping of atoms molecules. In particular, spontaneous light force, Doppler cooling of a two-level atom, sub-Doppler cooling, stimulated light force, magneto-optical trap, pulsed traps will be discussed. Optical manipulation of larger objects (nano- and microparticles) will be considered on an example of the optical tweezers. Finally, the problems of optical trapping of metallic nanoparticles will be revisited.

**Stefano BELLUCCI****QUALIFICATIONS  
AND EMPLOYMENT****Position:** First researcher**Professional affiliations:** INFN.**Field of Your interests:** Nanotechnology.**PERSONAL INFORMATION****WORK EXPERIENCE:**

Dr. Prof. habil. Stefano Bellucci obtained in 1986 his Ph. D. in Physics of elementary particles at SISSA, Trieste. He worked as Research Associate at Brandeis Univ., Waltham, MA, USA (1983–1985); as visiting researcher at M.I.T., Cambridge, MA, USA (1985–1986), at Univ. of Maryland, USA (1986–1987), at Univ. of California at Davis, USA (1987–1988). He was appointed as a Tenured Researcher (Research Staff) at INFN (Istituto Nazionale di Fisica Nucleare) Laboratori Nazionali di Frascati (LNF) in 1987. He was appointed as INFN First Researcher (Senior Research Staff) in 2005. He received by Italy Ministry of University in 2013 the habilitation as Full Professor in Theoretical Physics of Fundamental Interactions and the habilitation as Full Professor in Theoretical Condensed Matter Physics. He coordinated (1999–2002, 2011–2015) all LNF theoretical physics activities.

**EDUCATION AND TRAINING**

PhD in Physics 1986 SISSA Trieste, Italy.

**Lecture title:** Tunable Microstrip Attenuators and Patch Antenna based on graphene.

**Lecture abstract:** Recently graphene got a lot of attention for its potential use in microwave applications owing to its tunability properties. Graphene changes its resistance values from very high values to very low values upon the application of a voltage bias. This is particularly interesting in the design of microwave and millimeter wave components and structures. The use of few-layer graphene (FLG) is particularly interesting due to its ease of production and low cost. The ease of production and low cost of the graphene flakes however does not affect its tunability properties.

There are several possible topologies for designing tunable attenuators based on FLG flakes. FLG flakes are put in between a microstrip line. The microstrip line is connected to a voltage network analyzer on both its ports. Bias tees are used to bias the FLG flakes from either side. Increasing the bias voltage through the bias tees reduces the graphene resistance thus increasing the transmission through the microstrip line.

Another possible topology for the design of tunable microwave attenuator is by using grounded vias on either side of the microstrip line. These vias are symmetrically placed on either side of a microstrip line. The microstrip line and the vias are separated from each other by the help of FLG flakes. When biased, the grounded vias short out the microstrip line reducing the transmission through the microstrip line. Such a configuration results in better tunability with a comparatively narrower bandwidth.

FLG flakes can also be used in the design of tunable patch antennas. A patch antenna is connected to a shorted stub on its radiating edge through the FLG flakes. Biasing the FLG flakes reduces their resistance thus increases the impact of the stub on the patch antenna. This results in an elongating effect of the patch antenna thus shifting the radiating frequency. Varying the applied bias voltage results in varying the radiating frequency.

The interesting properties of graphene can be exploited in designing several other kinds of microwave structures ranging from tunable phase shifters to matched load circuits among several others. Thus it has the potentiality of revolutionizing the future of microwave structures.



**Eugene BORTCHAGOVSKY**

**QUALIFICATIONS  
AND EMPLOYMENT**

**Position:** Head of a laboratory, senior scientist.

**Professional affiliations:** Institute of Semiconductor Physics of NASU.

**Field of Your interests:** plasmonics, near-field optics, energy transfer, ellipsometry of nanostructures.

**PERSONAL INFORMATION**

**WORK EXPERIENCE:**

Expertise in ellipsometry, near-field optics, tip-enhanced Raman scattering.

Employment – V. Lashkarjov Institute of Semiconductor Physics of the NAS of Ukraine;

Contracts: Masaryk University (Brno, Czech Republic);  
Institute of Physics of CZ AV (Prague, Czech Republic);  
Westfälische-Wilhelms Universität (Münster, Germany);  
Istituto per la Microelettronica e Microsistemi CNR (Lecce, Italy);  
Quinsland University of Technology (Brisbane, Australia);  
Johannes Kepler University (Linz, Austria);  
ETH (Zurich, Switzerland);  
Technical University (Chemnitz, Germany).

**EDUCATION AND TRAINING**

2016 – Dr. of Sciences in Physics, Institute of Physics of the NAS of Ukraine;

1991 – PhD, Moscow State University;

1982 – MSc., Moscow Institute of Physics and Technology.

**Lecture title:** Ellipsometry of nanostructures on a surface.

**Lecture abstract:** Ellipsometric investigations of nanostructures on a surface have peculiarities created by two-dimensional character of such a structures. As the result, interactions along and across the surface are different producing effective optical anisotropy of such a structures. The situation is even more complicated because of the interaction of nanoobjects with the surface. These reasons do not allow to apply Lorentz sphere formalism for the fields averaging in heterogeneous nanostructure producing deviation of optical properties of such a structures from results given by standard 3D models of effective-medium approximation. These problems will be discussed and examples of ellipsometric investigations of both random and ordered nanostructures on surfaces will be presented. It is shown that polarization properties of light can give macroscopic information about microscopic interparticle interactions as well as ellipsometry allows to monitor behavior of modes localized on the layer of nanostructures and to register interactions of such a modes.





**Vladimir KORZH**

**QUALIFICATIONS  
AND EMPLOYMENT**

**Position:** Visiting professor.

**Professional affiliations:** International  
Institute of Molecular and Cell Biology.

**Field of Your interests:** Developmental  
biology, zebrafish, embryo toxicity, FCS,  
nanomaterials.

**EDUCATION AND TRAINING**

1976 – BSc, Dep. Biol. Sciences, Kiev State University

1981 – PhD, Koltsov Institute of Developmental Biology, USSR Academy  
of Sciences.

**Lecture title:** Zebrafish as useful in vivo model for nanomaterials  
embryotoxicity and disease treatment.

**Lecture abstract:** Since relatively recently zebrafish embryos started to be used to evaluate embryotoxicity and various physico-chemical properties of nanomaterials. This made it a popular non-mammalian research model animal. While it is relatively easy to work with zebrafish some training is necessary to be able to set experiments correctly and put forward proper scientific questions. Zebrafish researchers usually highlight advantages of zebrafish embryos as a model system. But what about their disadvantages? This lecture will cover various aspects of developmental biology of zebrafish and highlight its applications in analysis of nanomaterials.

**Nataliya STOROZHYLOVA**

**QUALIFICATIONS  
AND EMPLOYMENT**

**Position:** PhD (defending in September 2017).

**Professional affiliations:** University of Santiago de Compostela (Spain)  
University of Nantes (France).

**Field of Your interests:**

Nanotechnology, pharmacy,  
nanomedicine, glycochemistry and glycobiology.



**Lecture title:** New potential nanotechnology-based therapies for the treatment of rheumatoid arthritis.

**Lecture abstract:**

The design, development and in vivo evaluation of a novel injectable biodegradable drug delivery system, composed of in situ hydrogel combined with nanocapsules carrying lipophilic anti-inflammatory drugs, for prolonged intra-articular residence time and controlled drug release.



## Andrey KADASHCHUK

### QUALIFICATIONS AND EMPLOYMENT

**Position:** Senior Scientist (1993-to date);  
 Guest professor (Feb. 2017 – May 2017);  
 Guest professor (Jan. 2016 – Apr. 2016);  
 Guest professor (Jan. 2015 – Apr. 2015);  
 Guest professor (Feb. 2017 – May 2017);  
 Guest professor (Jan. 2014 – Apr. 2014);  
 Guest professor (Jan. 2013 – May 2013);  
 Guest professor (Dec. 2011 – Feb. 2012);

Guest professor (Nov. 2010 – Jan. 2011);  
 Guest professor (Nov. 2009 – Jan. 2010);  
 Guest professor (Sep. 2008 – Nov. 2008);  
 Guest professor (Sep. 2007 – Nov. 2007);

### Professional affiliations:

Institute of Physics of the NAS of Ukraine, Kyiv, Ukraine; IMEC  
 International;  
 Department of Large-Area Electronics, Leuven, Belgium;  
 Technical University of Darmstadt, Institute of Materials Science,  
 Darmstadt, Germany;  
 Philipps-Universität Marburg, Germany.

**Field of Your interests:** Eelectronic properties of thin-film organic and oxide semiconductor materials, organic semiconducting nanostructures and their applications as active media in FET, PV, and LED devices. Thin-film flexible electronics.

### PERSONAL INFORMATION

#### WORK EXPERIENCE:

- Study and modeling of the charge-carrier transport and trapping in organic optoelectronic device materials and nanostructures, as well as in thin-film amorphous oxide semiconductors.
- Gaining insight into excited states physics and exciton processes/migration, the charge-carrier trapping phenomena in semiconducting polymers, low molecular weight organic films and organic nanostructures.
- Physics of thin-film flexible electronic devices.

**EDUCATION AND TRAINING**

MS in Physics, Graduated from the Department of Physics of Kyiv State University in 1984.

Ph. D. in Physics, Institute of Physics, National Academy of Sciences of Ukraine, 1989.

Post. Doc. fellowships at TU-Darmstadt, Germany (2003–2004) and at IMEC, Belgium (2005–2006).

**Lecture title:** Modern trends in nanoelectronics and ultra-thin-film flexible electronics.

**Lecture abstract:** Integrated circuits (called also as "microchips") are at the heart of modern electronic devices (computers, smartphones, different electronic household appliances, etc.), which have nowadays penetrated every aspect of our lives. Downscaling is the dominant trend in microelectronics for more than 50 years, which implies creation of increasingly smaller constituting elements – transistors. The number of transistors in microchips doubles approximately every two years. This is a key to make electronic devices increasingly faster, cheaper and energy more efficient. The most advanced commercial microchips consist of several billions of tiny transistors with extremely small feature size of 10 nm as achieved now for processors and 7 nm for memories. This remarkable achievement truly means a transition from microelectronics to nanoelectronics and presents the widest practical realization of nanotechnologies as for today. In this lecture, I will present an overview of modern trends in nanoelectronics technology, relevant physical aspects as well as some corresponding innovations with particular focus on the Internet-of-Things (IoT) – a new increasingly growing topic. Furthermore, a new generation of electronics – the so-called thin-film flexible electronics will also be discussed in details including its impact on IoT implementation perspective.

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НАУКОВЕ ВИДАННЯ

**The International Summer School  
“Nanotechnology : from fundamental research to innovations”**

Book of abstracts of young scientists and lectures  
of the International Summer School  
(August 19 – August 26, 2017)

Book of abstracts is published in authors edition, without modifying  
by the Organizing Committee

Head of local Committee and Secretary International Summer School:  
Dr. *O. M. Fesenko*, Institute of Physics of the NAS of Ukraine

Design and layout: *Volodymyr Havlo, Eurosvit*

Technical support in the course of the International conference (NANO-2017).  
Junior Researchers of the Institute of Physics of the NAS of Ukraine A. A. Yaremkevych  
(media assistance) and Y. S. Kifiuk (sound equipment and photo report), Leading  
Engineers of the Institute of Physics of the NAS of Ukraine H. R. Cheriopkina  
(registration support), V. V. Kavelin (informational and transportation support),  
O. P. Budnyk (registration of participants and excursions), S. V. Kovalchuk (registration  
of participants and transportation), Dr. Khalavka Yuriy (General questions) and Mrs.  
O. Tynkevych (General questions), V. Vovk (General questions).

Здано в набір 01.08.2017. Підписано до друку 08.08.2017. Формат 60х90/16.  
Папір крейдяний. Гарнітура Таймс. Друк офсетний. Умовно друкованих аркушів  
6,48. Умовно фарбовідб. 6,72. Зам. 8.

Свідчення про внесення до Державного реєстру видавців,  
виготівників і розповсюджувачів видавничої продукції  
серія ДК № 1185 від 29.12.2002 р.

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Richard Feynman was the first scientist to suggest (in 1959) that devices and materials could someday be fabricated to atomic specifications. "The principles of physics, as far as I can see, do not speak against the possibility of maneuvering things atom by atom." This concept was expanded and popularized in a 1986 book *Engines of Creation* by K Eric Drexler, who applied the term nanotechnology to Feynman's vision.

Nanotechnology is the engineering of functional systems at the molecular scale.

What qualifies as "nanotechnology" today is basic research and development that is happening in laboratories all over the world. "Nanotechnology" products that are on the market today are mostly gradually improved products (using evolutionary nanotechnology) where some form of nanotechnology enabled material (such as carbon nanotubes, nanocomposite structures or nanoparticles of a particular substance) or nanotechnology process (e.g. nanopatterning or quantum dots for medical imaging) is used in the manufacturing process.

The term "nano-technology" had been coined in 1974 by Norio Taniguchi to describe semiconductor processes involving control on the order of a nanometer.

Nanotechnology refers to manipulating the structure of matter on a length scale of some small number of nanometers, interpreted by different people at different times as meaning anything from 0.1 nm (controlling the arrangement of individual atoms) to 100 nm or more (anything smaller than microtechnology).

