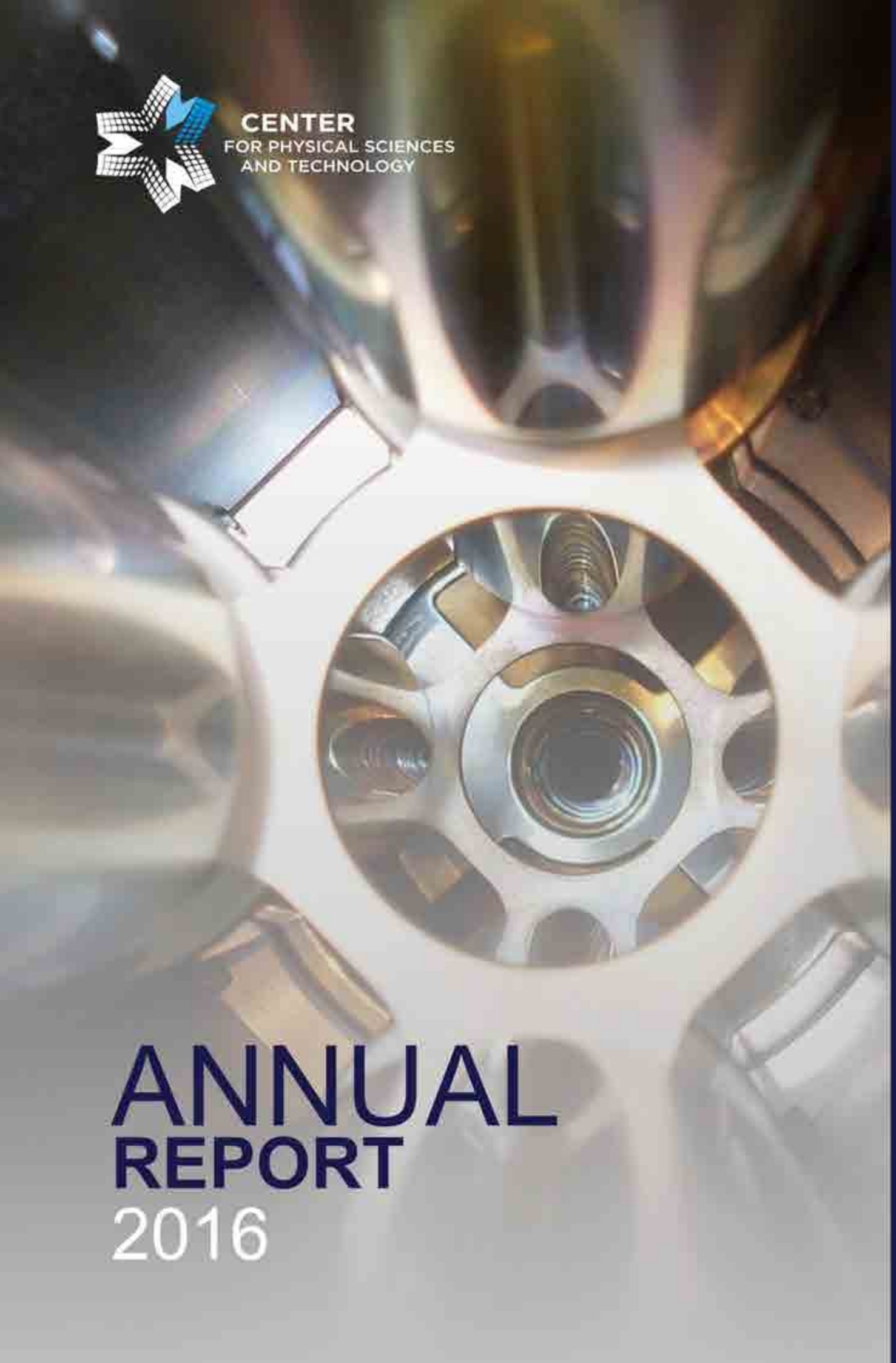

CENTER
FOR PHYSICAL SCIENCES
AND TECHNOLOGY

ANNUAL REPORT 2016

MODERN PATHS TO INNOVATIONS

Starting at Sunrise

It was a versatile start in a new geographical place at Saulėtekis (Sunrise) valley. The year 2016th completed our movement into contemporary building decorated by graphene-shaped windows and equipped with new facilities containing modern technological infrastructure. This change required nearly 10 years of thorough preparation: starting from definitions of scientific trends, evaluation of scientific resources and considerations on technological backgrounds; continuation with writings of feasibility studies and investment projects and, finally, careful installation of the newest equipment, precise accommodation of all technical services and building a managing system in a smart new environment of the National Centre for Physical and Technological Sciences.

The official opening date is the 15th March 2016.

President of the Republic of Lithuania Dalia Grybauskaitė, the Prime Minister Algirdas Butkevičius, and Jose Angel Gurria, General Secretary of the Organisation for Economic Co-operation and Development (OECD), have started the opening ceremony with their welcoming speeches. Delegations of the European Commission, CERN, MPs, and Ministers of the Republic of Lithuania, Diplomatic Corps, City Mayors and many other honorable guests have joined this exciting celebration.

The 15th March 2016 marks an important milestone in evolution of our Center. Moreover, it opens a novel avenue for Lithuanian science and technology providing qualitatively new facilities to create progressive synergies between the institutions situated in the neighbourhood, first of all, Vilnius University and Vilnius Gediminas' Technical University.

We are deeply convinced that modern technological facilities currently available at the Center will accelerate the quality of science and innovations, expand the scientific research for the development of high-tech business and encourage the birth of an advanced generation in high-tech industry.

We have new facilities, hence, we need creative, efficient and stimulating style of activities. We should proceed further as a promoter of bridging applied research and high-tech business via international and national projects, patents, licensing and comprehensive know-how based on our scientific experience.

We need international atmosphere inside the Center. We need acceleration in international relations-based modern trails to innovations. The Center is built on creative energy, inexhaustible enthusiasm and permanent drive of its people.

This Annual Report emphasizes the most interesting results obtained in science and technology, captures the breakthrough in projects and presents the numbers illustrating main achievements. The Report also features the essential events in the Center, shows the financial side of activities and last, but not least, highlights the Winners of the 2016th year and other people that allow us running strong in this interesting scientific journey.

Gintaras Valušis
Director of the Center

Fizinių ir technologijos mokslų centras (FTMC)

Center for Physical Sciences and Technology

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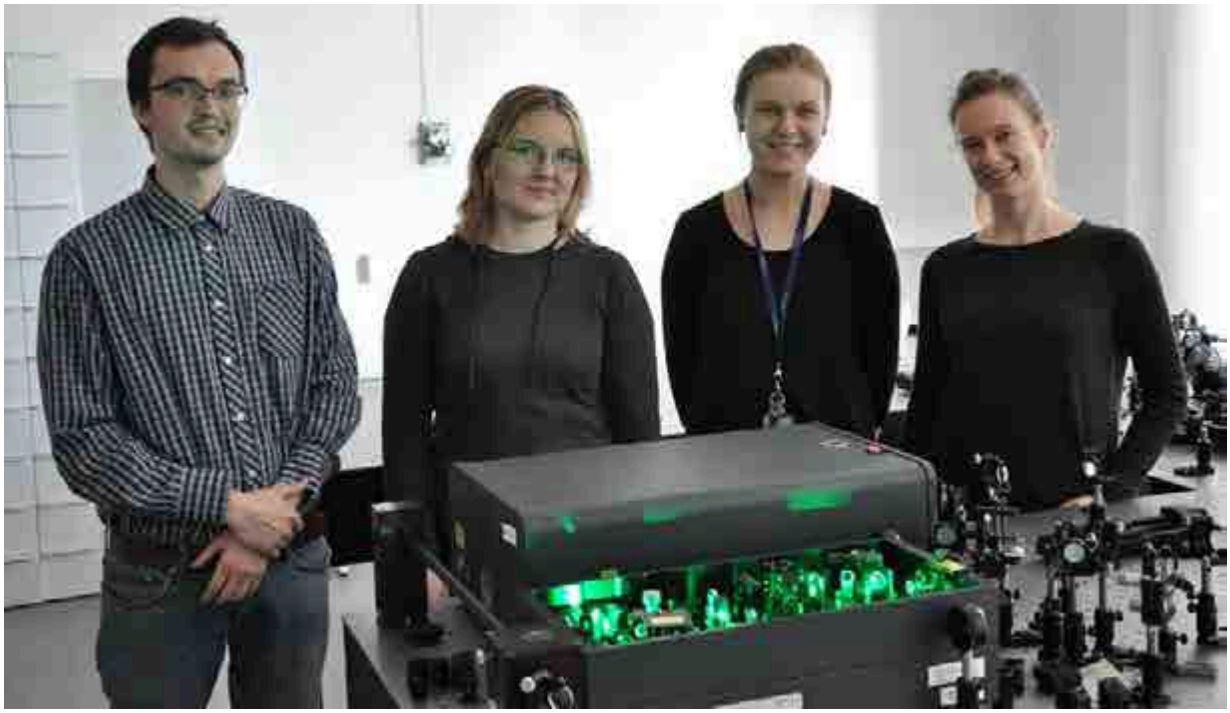
Optoelectronics



Semiconductors for the light technologies

Optoelectronics is widely recognized as one of the Key Enabling Technologies of the future. At Optoelectronics Department this field of research is developed in two main directions: i) epitaxial growth technology of semiconductor structures and devices for mid- and far-infrared spectral ranges and ii) terahertz frequency range components, systems, and applications. Moreover, the Department operates a most comprehensive set of standard optical characterization techniques that is intensely exploited also by other Lithuanian research groups and companies.

There are many paths you can go down when striving to improve device performance. One option is to keep it simple and try to improve the quality of the production processes, such as optimising the growth of the epi-ready wafer. This can pay dividends, particularly if the class of device is not well established. But by far the most radical route is to dispense with a mature material system, and adopt one that is yet to be tried and tested. That's what a team of FTMC researchers is doing, developing optoelectronic semiconductor components based on bismuth alloys, rather than standard A3B5 compounds. This effort has had to start from scratch, developing models to understand device behaviour and establishing appropriate growth conditions before it is even possible to try and fabricate the first devices. One attractive attribute of bismide alloys is the behaviour of their energy gap: It decreases very rapidly with bismuth composition, allowing growth of telecom lasers on a GaAs substrate. Our research group is one of the world leaders in developing bismide based lasers, photodetectors, and terahertz components.

Terahertz (THz) radiation, which lies in the frequency gap between the infrared and microwaves, typically referred to as the frequencies from 100 GHz to 30 THz, has long been studied in fields such as astronomy and analytical science. However, recent technological innovation in photonics and nanotechnology is now enabling THz research to be applied in many more sectors. THz imaging holds promise for a multitude of applications from biomedical imaging to the inspection of semiconductor devices. At the Optoelectronics Department we are active in investigating different THz spectroscopy and THz imaging applications, in developing novel optoelectronic THz frequency range components and systems. These are commercialized by two companies that have been started by the researchers of the Department.

Quantum decoration

Normally, GaAsBi layers with a larger Bi content contain numerous defects and show only weak photoluminescence (PL) signal. A group from the Optoelectronics Departments has found that after post-growth annealing this signal can increase drastically. This effect was accompanied by a nucleation of numerous Bi-rich nanoparticles that were randomly distributed and had various sizes. This year the group was investigating superlattices consisting of alternating GaAsBi/AlAs layers. AlAs layers were serving both as barriers for electrons and for Bi out-diffusion. Regular structures with GaAsBi quantum wells decorated by Bi nanocrystals were observed after thermal annealing. It has been shown that nanocrystalline bismuth is not semi-metallic anymore, but becomes a semiconductor with a strong zero-dimensional quantum confinement. The Bi quantum dots, displaying a strong PL in technologically important 1.55 mm wavelength range, can be prospective for light-emitting devices produced using a mature GaAs material platform.

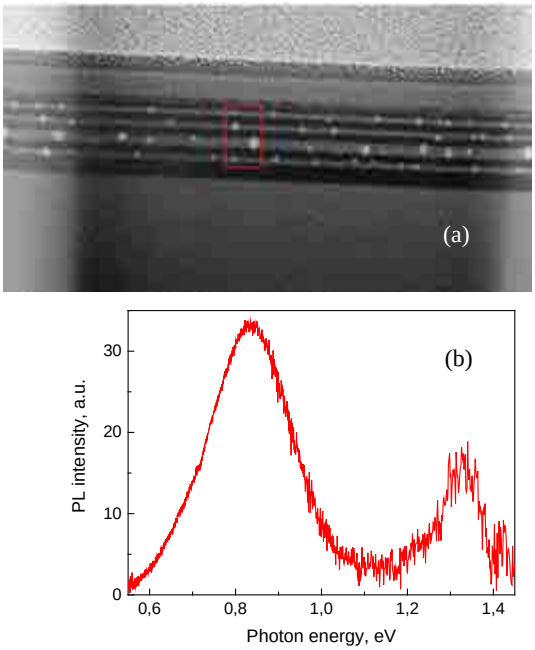


Fig. 1. (a) Transmission electron microscopy image of GaAsBi/AlAs superlattice. Bright spots are Bi nanocrystals. (b) Room temperature PL spectrum of this superlattice.

Beyond suspicion

In this work a compact THz imaging system was developed. To ensure small dimensions of the system, thin diffractive optics were developed for efficient THz beam focusing at a frequency of 584 GHz. A zone plate lens with a diameter of 16.5 mm and a 10 mm focal length was fabricated on a 30 µm thick metal foil by laser ablation technique. The lens was designed to have a high numerical aperture of about 0.6 required for tight focusing of THz radiation. Imaging of high resolution target revealed about 25% increase in spatial resolution as compared to commercial off-axis parabolic mirrors. Developed THz imaging system enhanced with novel terahertz optics was applied for biomedical microscopy applications. For this purpose, the dehydrated human colon tissues were imaged. The THz imaging was used as a tool to distinguish suspicious areas of neoplastic tumor-affected tissues by comparing them with non-neoplastic controls.

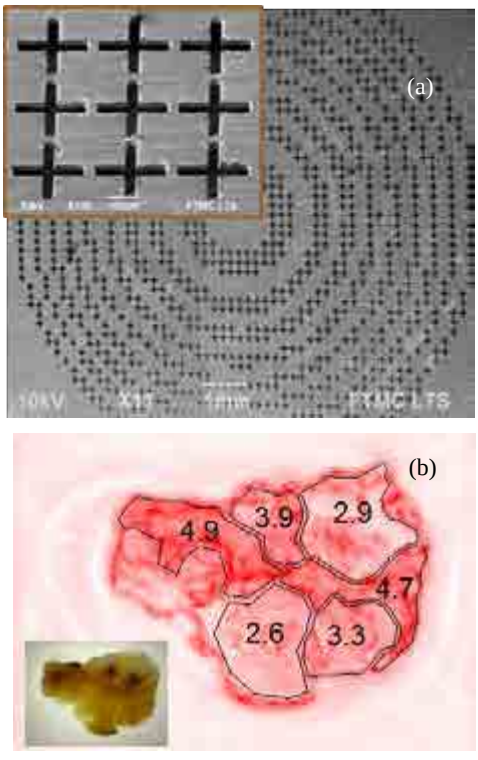
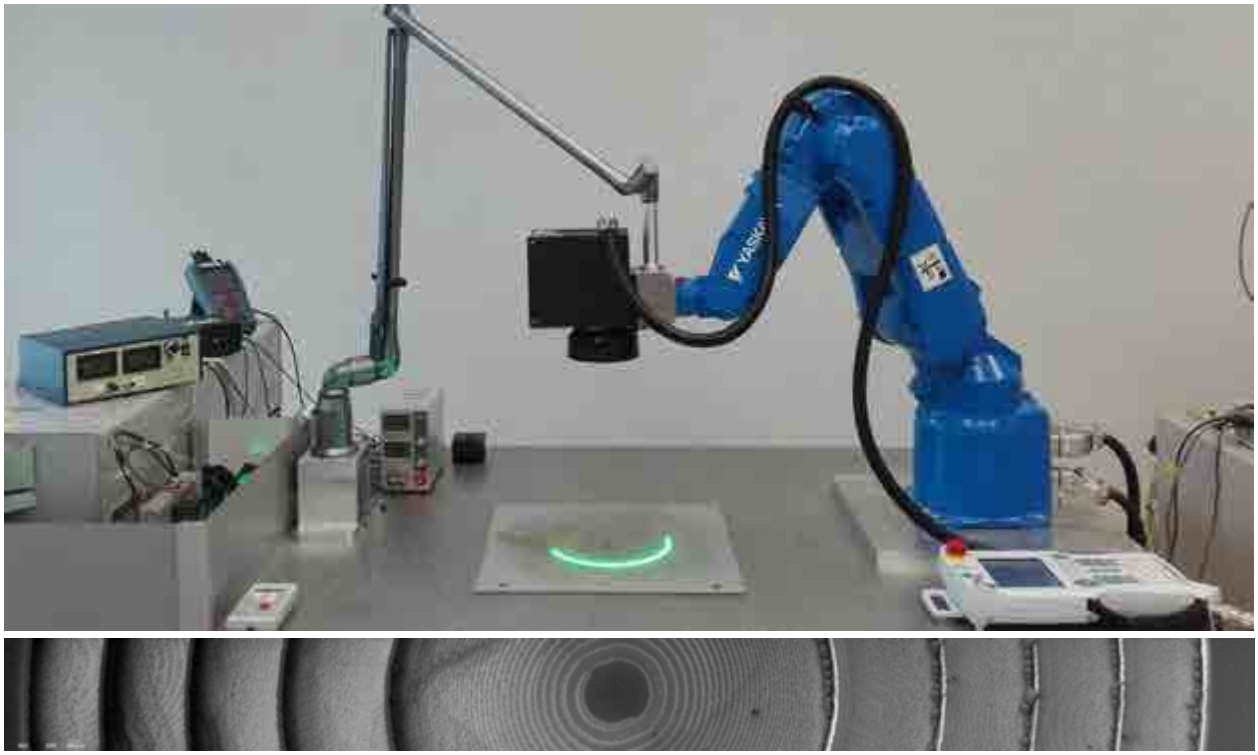


Fig. 2. (a) Terahertz zone plate lens and (b) the image of adenocarcinoma created by using this lens. A number inside each region presents the average value of THz absorption.

Laser technologies



Optical coatings, solid-state and fiber lasers, laser material processing and nanophotonics

Laser technologies are becoming a commodity in many areas of production as well as installed into consumer products. The Department of Laser Technologies with its six laboratories covers significant part of the photonics related activities, ranging from new discovered effects to laser machines, and stepping through all technology readiness levels. The smart optical coatings developed in the Laboratory of Optical Coatings convert the pieces of glass into valuable products able to control spectral and temporal properties of the light. New laser sources, under development in the Fiber Laser and Solid-State Laser Laboratories, that are based on tiny but smart fibres or active bulk crystals provide not only a new wavelengths of coherent radiation, but high peak power, ultra-short pulses and controlled wave front as well. Combining of the coherent beams makes the lasers even more powerful.

The scope in material processing using ultrashort pulse lasers includes the investigations of the laser-matter interaction as well as hardware development in a new Laboratory of 3D Technologies and Robotics. Thin film scribing for photovoltaics, efficient surface texturing utilizing laser beam interference, glass processing with lasers, nano-textures decorated by nanoparticles, novel processes for electroless plating of laser modified polymers, laser-induced transformations in graphene-like materials make up the main working topics of the Laboratory of Laser Microfabrication Technologies in 2016.

When the structure dimensions are smaller than light wavelength, new effects arise. The Laboratory of Nanophotonics deals with sub-wavelength structures, in this way enhancing interaction of photon propagating in micro-ring resonators with environment. This allows us to construct sensitive tools for sensing applications. Large group of scientists, PhD students and engineers work together in laser-related fields. Their tight collaboration with colleagues from other departments of FTMC (Optoelectronics, Physical Technologies, Nanoengineering, Organic Chemistry, Catalysis, Electro-chemical Material Science, Characterization of Material Structure) facilitates the progress in laser physics and applications.

Optimization of laser induced damage threshold (LIDT) in chirped mirrors

LIDT behaviour as a function of electric field strength distribution inside chirped multilayer coatings such as GTI and CM was analysed. Data confirmed that limiting factor for higher LIDT values is intrinsic damage of H material and/or H-L layer interface (Fig. 1b). It was experimentally demonstrated that optimization by redistribution of electric field in CM can lead to increased resistance to laser irradiation by at least a factor of 2 (Fig. 1c). Further layer design optimization of electric field by reallocating electric field maxima on L material layers is, most likely, possible as damage occurred only on H layers. Suggested CM design improvement could increase reliability and LIDT performance of both CM elements, and high power systems they are used in.

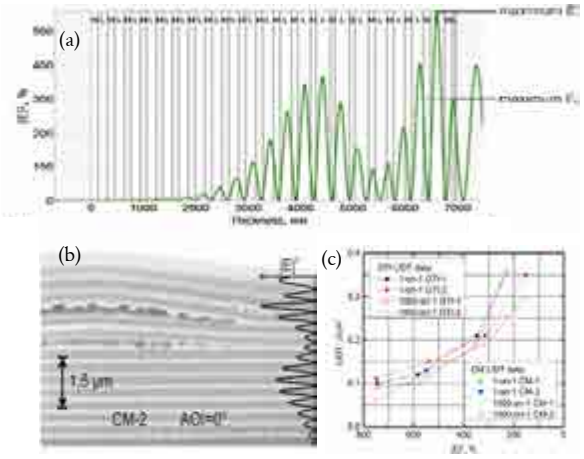


Fig. 1. (a) Electric field strengh inside CM. (b) Cross-section of damaged site in CM. (c) The dependence of LIDT on electric field inside multilayer structures.

Beam combining of fiber lasers by noncollinear frequency conversion

The proof-of-concept of pulse multiplexing and beam combining of four pulsed Yb-doped fiber lasers by non-collinear frequency up-conversion in an LBO crystal was experimentally realized. An overall conversion efficiency of 51% and up to 29 W average power in a combined 532 nm beam were achieved. These results correspond to an improvement by a factor of 2 compared to the average power extracted from a single fiber amplifier. The pulse peak power achieved in our setup was as high as 150 kW, which is quite a high limit. The second-order nonlinear interaction is a process without quantum defect, so the only channel for heat deposition is absorption which is very low for LBO crystals. This permits the upscaling of the method to multi kW range.

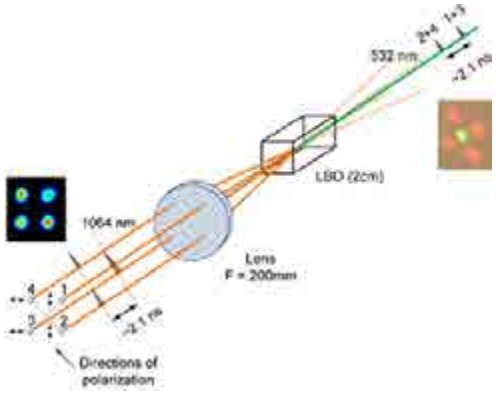


Fig. 2. Setup for beam combining by noncollinear sum-frequency generation. Insets: lateral intensity distribution of four fundamental beams before the focusing lens and beams after the crystal.

Femtosecond wavelength-tunable OPCPA system based on picosecond fiber laser seed and picosecond DPSS laser pump

A compact femtosecond tunable optical parametric chirped pulse amplification (OPCPA) system with a picosecond all-infiber seed laser and a picosecond DPSS pump laser was developed. A novel OPCPA front-end was constructed using a multi-channel picosecond all-in-fiber source for seeding DPSS pump laser and white light supercontinuum generation. Broadband chirped pulses were parametrically amplified up to 1 mJ energy and compressed to less than 40 fs duration. Pulse wavelength tunability in the range from 680 nm to 930 nm was experimentally demonstrated.

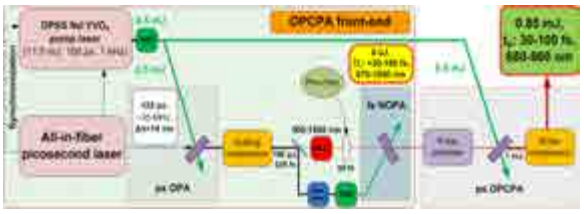


Fig. 3. Scheme of the fs wavelength-tunable OPCPA system. Multiple channel all-in-fiber ps-laser was used to seed DPSS pump laser and a non-collinear optical parametric amplifier (ps NOPA) to form pulses for white light supercontinuum (WLC) generation. WLC pulses were preamplified in femtosecond NOPA performing wavelength tuning, then stretched to picosecond duration, amplified in one stage OPCPA amplifier and recompressed.

Microring resonator with photonic crystal for refractive index sensing

Experimental and numerical analysis of a microring resonator, with an integrated one-dimensional photonic crystal fabricated on a silicon-on-insulator platform, shows its applicability in bulk refractive index sensing. The photonic crystal was formed by periodically patterned, partially etched cylindrical perforations which induced photonic bandgap narrower than the range of measurable wavelengths (1520–1620 nm). The microring operates in both air and dielectric bands, and therefore the sensitivities of the resonances on both edges of the bandgap have been investigated. Higher field localization inside the perforations for the air band mode leads to an increase in sensitivity.

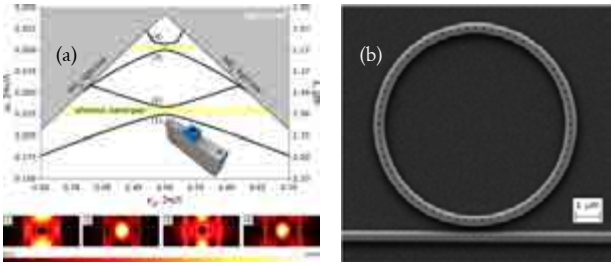


Fig. 4. (a) Band diagram of holey bend waveguide. The bottom panels show the distribution of electric field energy density of all four bands at $\kappa_x = 0.49$. (b) Scanning electron microscopy image of a fabricated microring resonator.

Bessel-like beam array generation using round-tip micro-structures and their use in material treatment

A novel and flexible strategy to create an array of the Bessel-like beams using the four-beam laser interference technique is presented. The generated beams show all fundamental features of the Bessel-like beams. Validation of the optical performance of these beams was demonstrated utilising the polymerised structures as a beam-shaping element in laser microprocessing. Different types of structures were fabricated in thin gold film, SZ2080 photopolymer and on ink-coated glass. All fabricated structures repeat the transverse intensity distribution of the Bessel beam. The dimensions and the periodicity of the manufactured structures perfectly fit into the range of terahertz waves. Therefore, the proposed method can be useful in the fabrication of terahertz metamaterials.

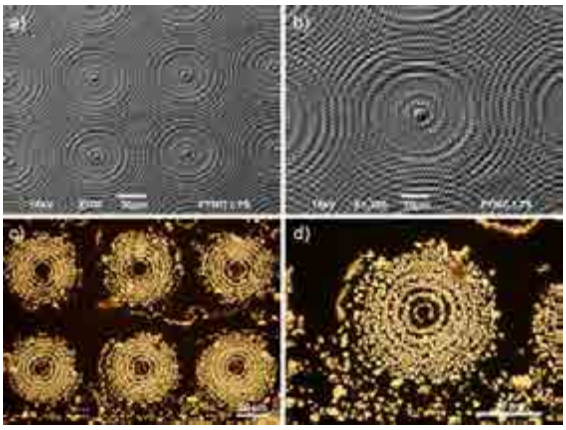


Fig. 5. Structures fabricated by using microaxicon-like structures as the beam-forming element: (a, b) SEM images of structures polymerised in SZ2080. (c, d) Optical microscope images of structures ablated in the thin gold film (~ 20 nm).

New processes for laser-induced electroless copper plating for MID

Moulded interconnect devices (MID) offer the material, weight and cost saving by integration electronic circuits directly into polymeric components used in automotive and other consumer products. Lasers were used to write the circuits directly, by modifying the surface of polymers followed by an electroless metal plating. A new composite material – the polypropylene doped with multiwall carbon nanotubes was developed for the laser-induced selective metallization. Mechanism of surface activation by laser irradiation was investigated in detail utilising pico- and nanosecond laser. A spatially selective copper plating was achieved with the smallest conductor line width of 22 μm at laser scanning speed of 3 m/s and the pulse repetition rate of 100 kHz.

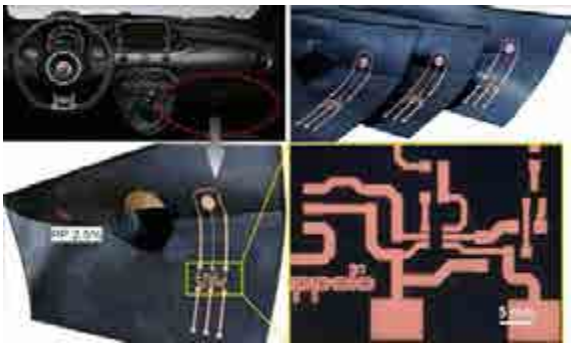


Fig. 6. Conductive tracks for a gloves box cover touch button demonstrator, using polypropylene doped with multiwall carbon nanotubes.

Laser cutting of glass with asymmetrical Bessel beam

Conventional processing tools of glass are facing serious challenges in terms of processing speed and quality. While nowadays most of the laser processing is dedicated for thin, especially chemically strengthened glass, there is still a need for a suitable processing technique for thick glasses. One of the most material-efficient and energy-efficient glass cutting techniques is to locally weaken the material along the cutting path by generating cracks or material modifications and then separate sheets by applying thermal or mechanical load. Bessel beams have very appealing properties (long non-diffractive propagation length and self-reconstruction) for processing of transparent materials. We demonstrate the possibility to cut glasses up to 5 mm thickness by applying Bessel beam induced modifications. The cutting process offers high cutting efficiency.

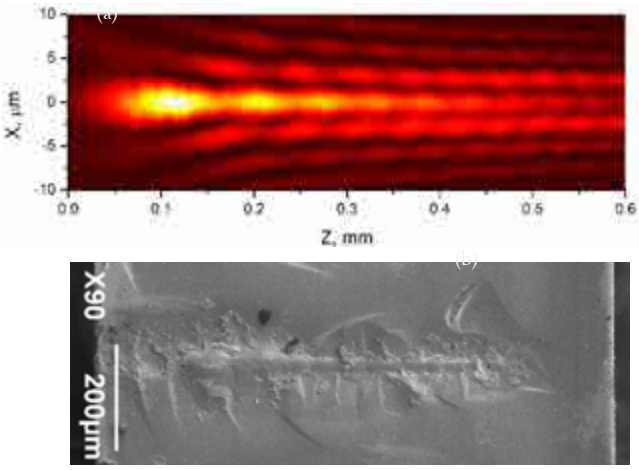


Fig. 7. (a) Intensity distribution in the XZ plane of the Bessel beam.
(b) Cleaved glass sample with laser-induced single-shot modification.

A method for evaluation of quality of electroless Cu deposition on a polymer after laser-induced selective activation

A novel colour-difference measurement method for the quality evaluation of copper deposited on a polymer is proposed. Laser-induced selective activation (LISA) was performed onto the surface of the PC/ABS polymer by using nanosecond laser irradiation and copper plated by using the electroless copper plating (ECP) procedure. The colour-difference of sample images after LISA and ECP procedures was found to be linearly proportional to the sheet resistance measured by using a four probe technique.

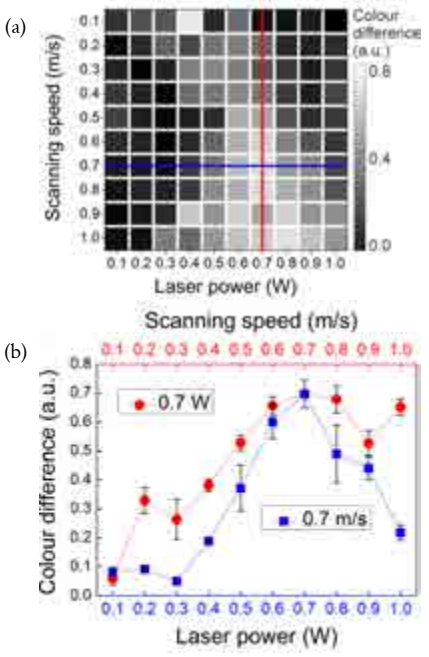
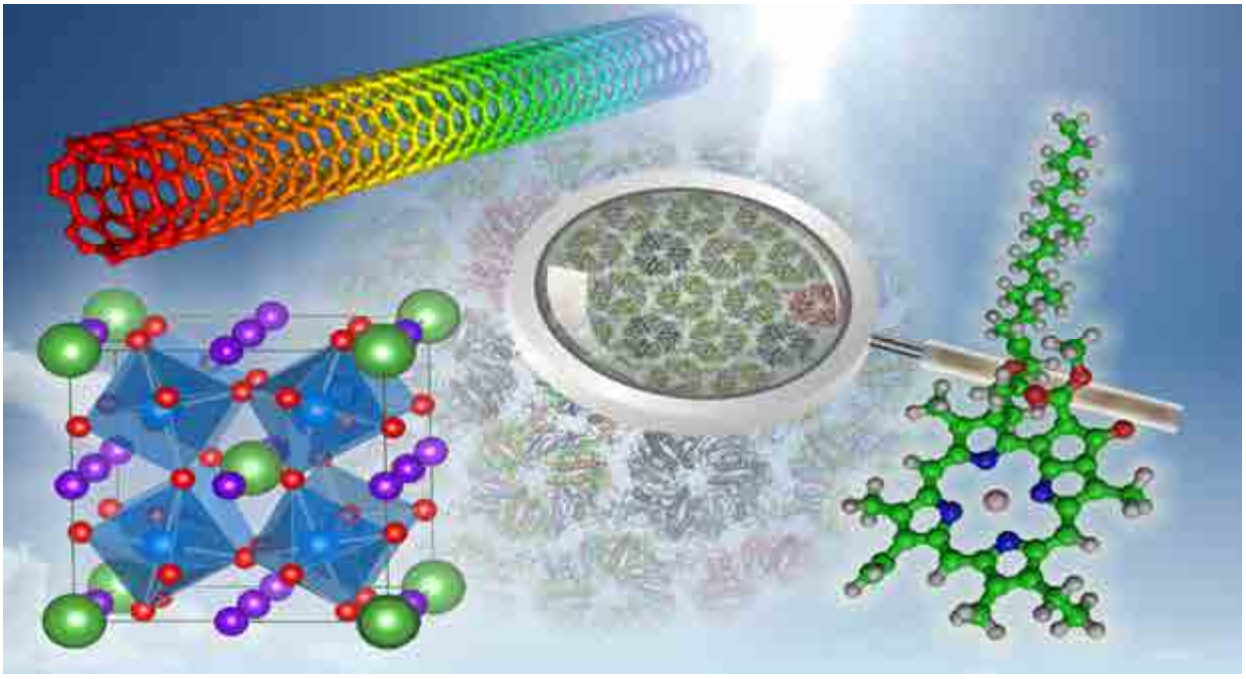


Fig. 8. (a) The map of colour difference between images after the LISA and ECP procedures at different laser powers and scanning speeds.
(b) Colour difference vs. processing parameters.

Molecular physics



Excitation dynamics and dissipation in natural and artificial molecular systems

Molecular systems, studied usually due to their biological relevance, recently started to show a strong potential for applications in technology and industry. Organic materials increasingly penetrate into electronics—the field that used to be totally dominated by the inorganic semiconductors in the past. Electronic devices such as organic light-emitting diodes, organic solar cells, or organic field effect transistors are often cheaper and more flexible, with quantitatively different properties. Unlimited variety of organic molecules as well as a broad range of technological fabrication abilities promise a wide spectrum of device characteristics. On the other hand, that raises requirements for a detailed understanding of molecular properties responsible for processes that take place in the molecular-based materials. Amazing functional characteristics and reliability of molecular systems created by Nature suggest operational principles that might be adapted for various man-made devices. Nonetheless, because of the complexity of natural systems, a blind mimicking usually does not work. Operational principles and device fabrication techniques, developed for inorganic materials, also cannot be directly transferred to molecular devices. Molecular systems necessarily involve a significant amount of nuclear dynamics, ranging from coherent nuclear vibrations at high frequencies to Brownian fluctuations or even proton transfer reactions in the molecular complexes. In addition to that, the molecular aggregates have multiple electronic excited states (excitonic states) that are responsible for the spectral properties and are involved in the photoinduced processes and reactions. All this complexity of the energetic arrangement has to be taken into consideration in order to enhance the efficiency of the molecular devices. The possibility to achieve this aim is well exhibited in natural molecular complexes. For instance, in photosynthesis the flexibility of the protein structure is a fundamental feature that probably has been utilized by Nature to select and optimize biologically relevant structural configurations. Studies of this type are carried out in the Department of Molecular Compounds Physics. Experience in experimental and theoretical approaches, obtained by studying numerous molecular systems, allows us to expect novel practical applications of the systems under consideration.

Multistep fluorescence decay reveals dissociation of geminate charge pairs in organo-lead trihalide perovskites

Despite rapid progress in the efficiencies of organo-lead halide perovskite solar cells which now exceed 20%, fundamental understanding of the perovskite properties ensuring high photovoltaic (PV) performance still lags behind. We elucidated the nature and initial dynamics of photo-generated charge carriers in methylammonium lead iodide perovskites by means of picosecond time-resolved photoluminescence spectroscopy at various temperatures (20–300 K). Our studies allowed us to separate geminate and non-geminate recombination processes and to show that geminate recombination dynamics is determined by the loss of spatial correlation between initially generated charge pairs.

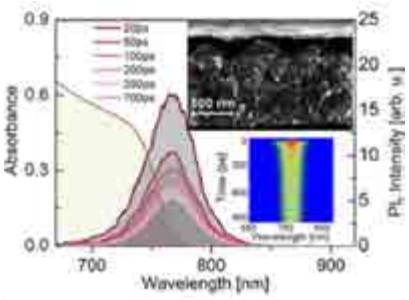


Fig. 1. Photoluminescence properties of $CH_3NH_3PbI_3$. Time-dependent photoluminescence spectra of $CH_3NH_3PbI_3$ perovskite films at room temperature, measured at different delay times after excitation. Insets show cross-sectional scanning electron microscope image of the film and visualization of the streak camera data.

Carrier photogeneration, recombination, and drift in carbon nanotube network

Charge carrier photogeneration, drift, and recombination in a network of enriched (6,5)-single-wall carbon nanotubes (SWNT), blended with Phenyl-C61-butyric acid methyl ester (PCBM), have been investigated in the films deposited on the interdigitated electrode arrays. Three distinct transient photocurrent components have been identified: the ultrafast component shorter than 2 ns attributed to the hole transfer within individual nanotubes, the intermediate component of several microseconds attributed to the hole transfer between neighboring nanotubes, and the longest component of several tens of ms attributed to electron transfer via PCBM. The hole transfer distance appears to be limited by gaps in the nanotube percolation network.

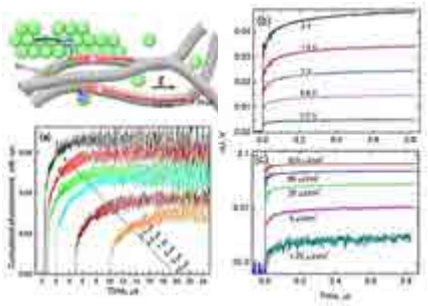


Fig. 2. Transient photocurrent in PCBM/SWNT blend. (a) Photocurrent kinetics, measured with time-delayed collection field technique at different extraction delay times; (b) photocurrent kinetics obtained at different constant applied voltages and (c) at different excitation intensities when applied voltage was 2 V.

Conformational dynamics in light-harvesting photosynthetic pigment–protein complexes

Fast excitation energy transfer within the light-harvesting antenna of the photosynthetic membrane, occurring on a timescale up to 100 ps, is modulated by the slow (micro-to-milliseconds) motion of the protein scaffold, resulting in the conformational switching of the pigment–protein complex between several spectroscopically and functionally different states. While single-molecule spectroscopy (SMS) allows us to directly observe this conformational protein dynamics via rapid fluctuations of fluorescence intensity during continuous illumination, time-resolved fluorescence measurements of the light-harvesting antenna, performed over wide temperature range and accompanied with theoretical simulations, can provide information about the molecular nature of each possible state.

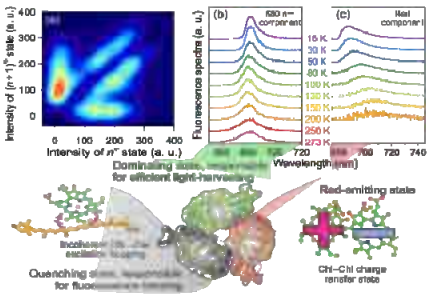
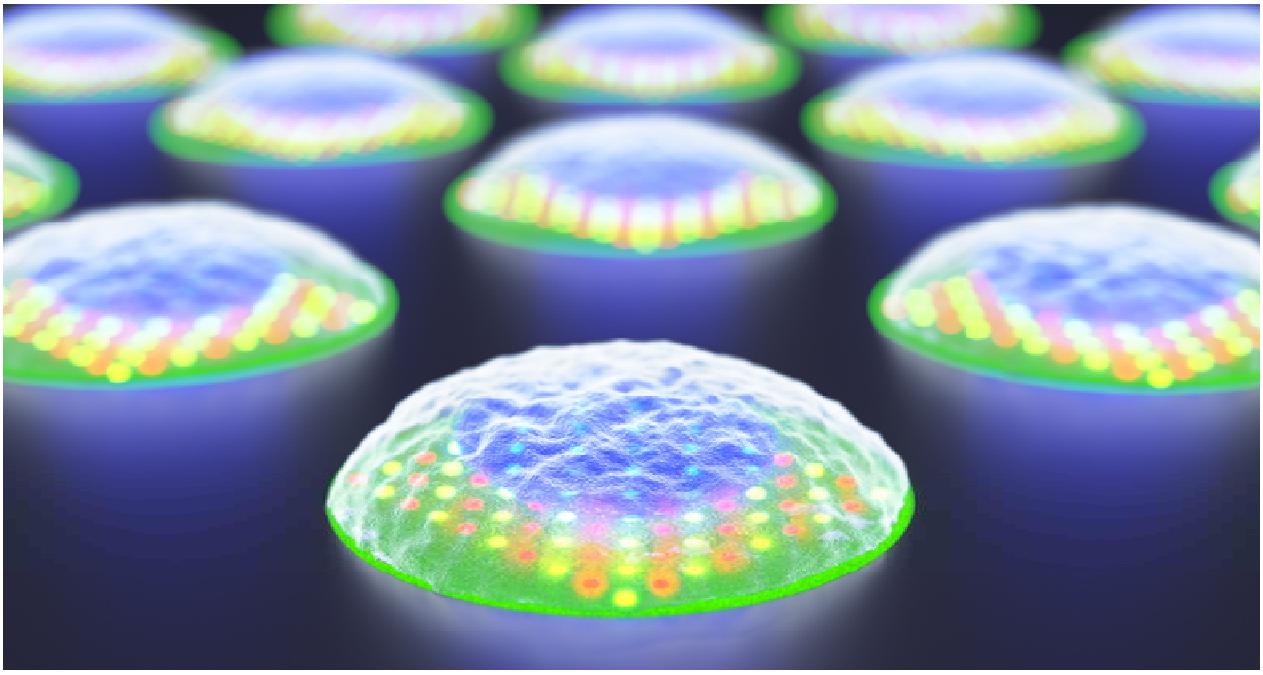


Fig. 3. Spectroscopic properties of the photosynthetic light-harvesting complexes. (a) Probabilities for the pigment–protein complex to switch between conformational states corresponding to different fluorescence intensities, obtained from SMS measurements. (b) and (c) Temperature dependence of the fluorescence spectra of two distinct conformational states, obtained by analysing data from the streak camera measurements, and their molecular mechanisms.

Nanoengineering



Fabrication and applications of nanostructures

Mission – new tools and processes for on-chip fabrication and integration of physical, chemical and biological nanoarchitectures.
Aims – establishment of reliable experimental platforms for biophysical studies of desired complexity: proteins, single cells and tissues, miniaturized sensor arrays.
Tasks – High speed nanolithography of functional patterning of soft (molecular) and solid surfaces, cell membrane-mimetic assemblies, nanobiochips for single cell analysis, micro/nanofabrication of hydrogel interfaces for tissue engineering, electrochemical and optical micro/nanosensors.
The activities of the Department of Nanoengineering are divided into three major subgroups:

Alternative nanofabrication. We are investigating nanometer-scale transport and assembly of molecules at interfaces to identify the physical principles for formation of molecular and hybrid architectures with controlled physical and chemical properties. Based on that, we are developing fabrication processes for rapid prototyping and small batch production. Recent examples include nanochips for single-cell level analysis of cytoskeleton, probing of cellular metabolism, or plasmonic sensing of protein-protein interactions.

Synthesis and functional modification of nanomaterials. We are employing organic synthesis for designing bi/multifunctional compounds that are used as building blocks of self-assembling structures. We are investigating in situ synthesis of nanostructures, e.g., by click-chemistry or electrochemical polymerization of conductive compounds.

Sensing and miniaturized analytics. We are developing localized surface plasmon resonance-active structures for on-chip detection of specific biomarkers (proteins). We have strong expertise in miniaturized electrochemical sensor systems for cell analysis, diagnostics and biosafety: from fabrication and characterization of microelectrode arrays to a complete portable device. We are pushing forward scanning probe technologies for characterization of molecular assemblies, soft materials and biointerfaces.

Nanometer-thick „foil“ for controlled release of biosubstances

Together with scientists from the University of Heidelberg we have established a new method for microscopic integration of bioactive or drug substances on the surfaces of implants, prosthesis, medical devices. It is based on stabilization and/or encapsulation of bioactive formulations pre-arrayed as microspots on the surface by contact transferring onto them a hydrogel-like “nanofoil”. The latter is composed of crosslinked PEG and extracellular matrix proteins, peptides. It acts as a delicate physical barrier for enclosing the bioactive substances, e.g. transfection mixtures, which after a certain delay time are accessed and taken up by cells and tissues.

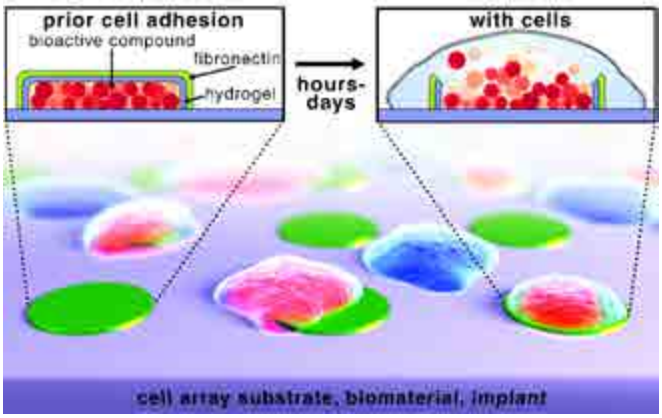


Fig. 1. Simplified schematic of the patented bioactive compound delivery assembly, explaining the principle of prolonged solid-phase transfection of adherent cells.
Once a cell settles on the micropattern, the latter releases the transfection mixture and starts the phenotype modulation programme.

New conducting polymers for electrochemical sensors

New conducting polymer composed of natural monomer riboflavin (vitamin B_2) was electrochemically synthesised and characterised. It was spectroscopically determined that the formed compound is polymerised riboflavin. The polymerisation goes via connection between rings I (N heteroatom from amide group) and III.
This polymer was applied for fabrication of the biosensors for hypoxanthine and glutamate. The latter was especially stable in comparison to those reported in the literature.

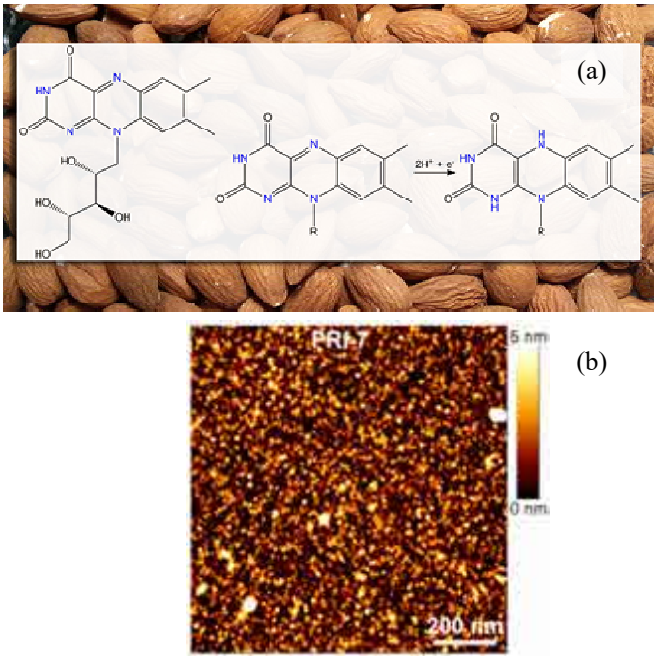
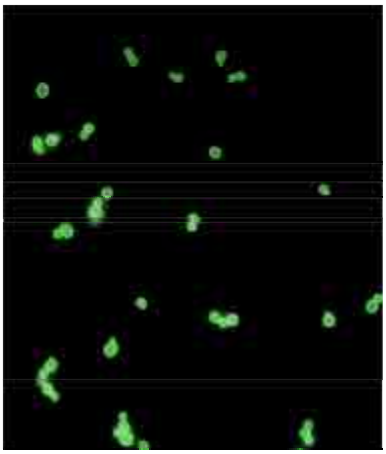
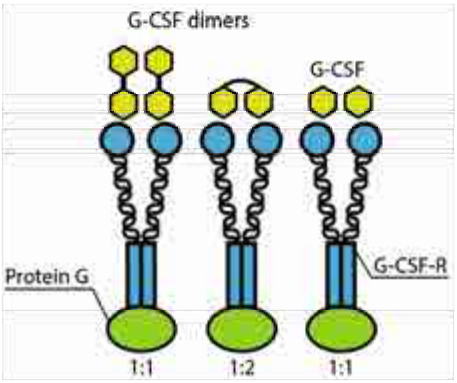
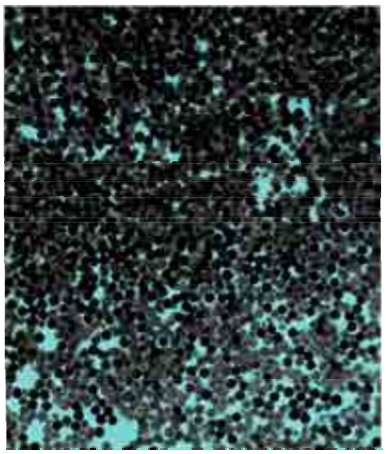


Fig. 2 (a) Chemical structure of riboflavin (vit. B_2) and its electrochemical reaction. The background depicts one of the sources of vitamin B_2.
(b) AFM image of obtained polymer.

Bio-nano technologies







Bio-sensor and living cell based technologies

The majority of electrochemical sensors and biosensors are based on chemical or biochemical structures selectively interacting with analyte. Depending on a type of a sensor, the role of such structures can be played by self-assembled organic and inorganic molecules, molecularly imprinted polymers, enzymes, antibodies, receptors, etc. Density functional theory and Monte Carlo simulations both are powerful tools to model and predict the assemblies of organic molecules on selected substrates. However, the incorporation of sensing and biosensing structures in analytical systems is still a challenging task that could be solved by proper application of π -π conjugated polymers. Many different methods of their synthesis are used, ranging from the basic chemical or electrochemical, up to the enzymatic, microorganism-based or microfluidics.

Biogenic and bioinspired microfluidic polymerization of pyrrole

Conducting polymers have attracted a lot of interest because of their applications in different fields of science and technology, e.g. as bionic organs and actuators in biorobotics or for modeling of cosmic dust in space science. Our resent research is focused on biogenic conductive polymer – polypyrrole, which was polymerized by bacteria *Streptomyces*. The observations revealed the structure of hollow polypyrrole microspheres from 10 to 25 μm in diameter. To control the process of their polymerization and formation of microspheres, the microfluidic device was developed. This device allows us to polymerize the pyrrole in situ by formation of microparticles at final stages of the process.

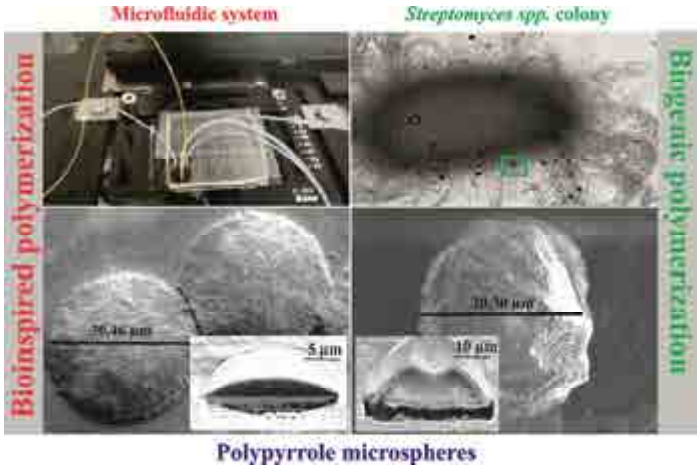


Fig. 1. Different methods of polypyrrole synthesis. (Left, above) Microfluidic system for microemulsion polymerization and (left, below) the microspheres obtained by this method. (Right above and below) *Streptomyces spp*. colony with polypyrrole microspheres. Insets: the cross sections of microspheres obtained by different methods.

Nanostructures for applications

2D Material technology for gas and photo-sensitive systems

Miniaturisation and integration of sensors into electronic systems requires new approaches in the key enabling technologies acceptable to combine commonly used semiconductor elements with appearing novel forms of 2D materials. We are developing original methods for assemblage of individual graphene sheets with the electronic components. We demonstrated that the parameters of electrical contacts in these combined components can be significantly improved by adequate annealing under controlled conditions. However, a mechanical manipulation of 2D sheets frequently is not acceptable for manufacturing of electronic devices. Therefore, we exploit the idea that formation of the stacked layers of 2D materials can also be carried out by direct synthesis of predictable number of sheets in the multicomponent structure. The "bottom-up" approach is acceptable for the layer by layer assemblage of vertical devices. As a part of this technology, we are developing the synthesis of MoS_2 layers on Si/SiO_2 substrate. By using the original CVD process based on sulfuring of ultra-thin metallic Mo films, we synthesized layered structure of MoS_2 which, depending on thickness of precursor Mo layer, contains from 1-2 to large number of atomic layers. The number of MoS_2 layers was detected by the Raman spectroscopy (see Fig. 1a). Aiming to combine the responses to light and gases in a single chip electronic system we developed an original approach to the surface texturing by the Cu-assisted etching. In Fig. 1b the p-Si surface is shown after one-step controlled etching. The experiments proved that the dimensions of the pyramid-like objects on Si surface can be intentionally changed by the etching conditions. By combining the 2D layers, ultra-thin metal oxides and surface texturing, we expect to create a novel type of hybrid detector for light controlled gas detection.

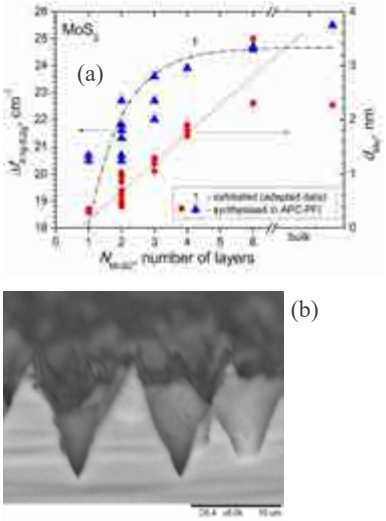


Fig. 1. (a) Frequency difference Δf between peaks A_{1g} and E_{2g} in Raman spectra versus number of MoS_2 layers synthesized by CVD using precursor Mo film of thickness d_{Mo}. (b) SEM image of pyramid-like textured Si surface intentionally modified by Cu-assisted etching.

Nanostructured materials for magnetic field sensing

Nanostructured manganite thin films exhibiting colossal magneto-resistance (CMR) phenomenon are promising materials for the fabrication of B-scalar sensors measuring high pulsed magnetic fields independently of field orientation. In collaboration with Vilnius university, we developed the pulsed injection MOCVD technology for the deposition of nanostructured (column-shaped crystallite, Fig.2a) $La_{1-x}Sr_xMn_{1+y}O_{3+\delta}$ (LSMO) films, which enabled to tune the phase transition temperature, resistivity and magnitude of MR. Aiming to increase temperature range of operation of magnetic field sensors, we introduced Mn excess in the films which gave the increase of the resistivity maximum temperature T_m by 20 K. The 15 % Mn excess in the films with Sr content $x \approx 0.18$ was found to increase the T_m from 250 K up to 270 K (see Fig. 2b). The room temperature MR was also found to be higher in comparison to films with $y = 0$. These results enables us to develop a novel CMR-B-scalar magnetic field sensor operating up to 70 °C temperature.

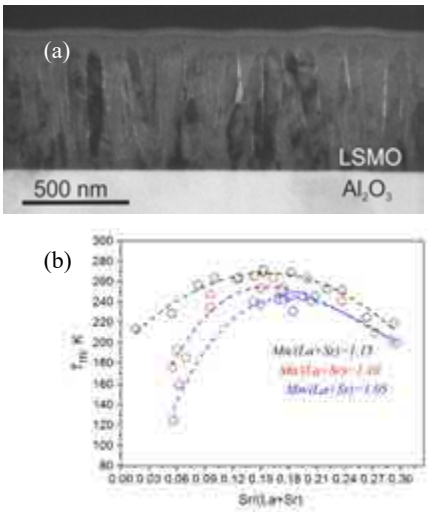
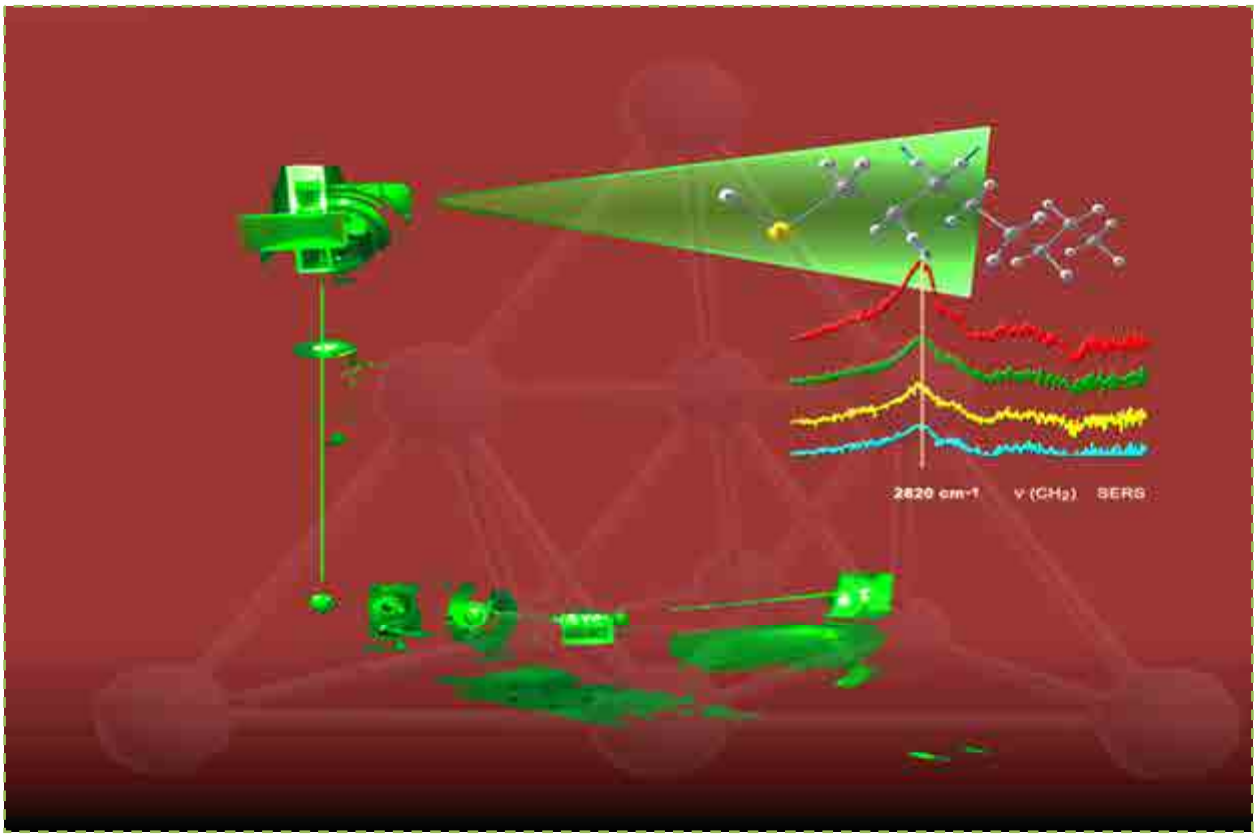


Fig. 2 (a) TEM image of nanostructured LSMO film grown on polycrystalline Al_2O_3 substrate. (b) Dependences of resistivity maximum temperature T_m of the films on Sr content x for different Mn excess y.

Spectroelectrochemistry



Spectroscopy of adsorption and electrochemical processes at a metal-solution interface

Electron transfer reactions, electrocatalysis, function of biomolecules, and corrosion processes critically depend on adsorption of organic molecules at metal surfaces. Bifunctional self-assembled monolayers (SAMs) are widely used for construction of surfaces with desirable properties. To predict and control the function of SAMs, molecular level understanding of monolayer architecture is required. We have used one of the most sensitive vibrational spectroscopic tools, surface-enhanced Raman spectroscopy (SERS) for in-situ probing the bonding, structure, and orientation of adsorbed molecules at Au, Ag, and Cu surfaces. In addition, reflection absorption infrared spectroscopy and sum frequency generation spectroscopy were used for analysis of electrochemical interface. The spectroscopic methods were coupled with first principle calculations and isotopic substitution approach. Spectroscopic experiments were conducted in-situ at controlled electrode potential. We have provided spectroscopic evidence for the interaction of the gauche conformer of adsorbed mercaptoethanol with the Au surface through both S and O atoms. The first principles calculations revealed shortening of the metal-oxygen bond upon hydrogen bonding of water molecule at the electrochemical interface to the OH group of mercaptoethanol. Vibrational spectroscopic evidence for formation of polymeric riboflavin film at Au electrode surface was provided.

Probing of water-induced structural changes in self-assembled monolayers on electrode surface

Water is required for biological function of tethered bilayer lipid membranes consisting of a lipid bilayer anchored by a mixed self-assembled monolayer (SAM) to an electrode surface. Water-induced structural changes in mixed SAMs and bonding with gold substrate were probed in situ by the isotope-edited SERS coupled with the first-principles calculations. The assignment of the bands was based on experimental analysis of deuterated 2-mercaptoethanol and quantum chemical modeling of adsorption complex consisting of Au cluster of 10 atoms. Evidence for the interaction of the gauche conformer with the Au surface through both S and O atoms was obtained from the analysis of the Au-S/Au-O vibrational mode near 303 cm^{-1}. First principles calculations of adsorption complex revealed shortening of the Au-O bond upon hydrogen bonding of explicit water molecule to the OH group of 2-mercaptoethanol (Fig. 1).

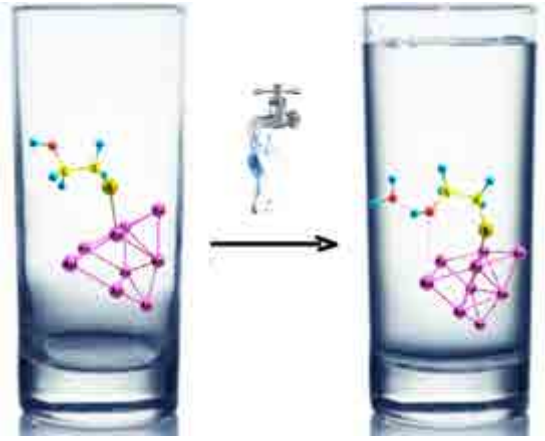


Fig. 1. Structures of surface model complexes with explicit water molecule in gauche and trans conformation optimized at the DFT-3BLYP/6-311++G(d, p) level for C, D, H, S, and O atoms and LANL2DZ with EPC for Au atoms.

Assessing the molecular structure of electropolymerized thin films at electrodes with vibrational spectroscopies

Structure of electropolymerized riboflavin was probed by Raman spectroscopy and reflection-absorption infrared spectroscopy (RAIRS) methods. Raman spectra have demonstrated that polymerized riboflavin exists in the oxidized form and it is formed on the basal plane of the high oriented pyrolytic graphite (HOPG). Both RAIRS and Raman spectroscopies data suggested that isoalloxazine ring III (Fig. 2) participates in the polymerization process. A broad feature near 1148 cm^{-1} visible in the RAIRS spectrum of polymerized riboflavin on the Au electrode was assigned to stretching vibration of the C-N bonds formed between the isoalloxazine rings during the polymerization process (Fig. 2). The most probable polymerization path goes via bonding of the N3 atom in ring III to the C6 atom in ring I.

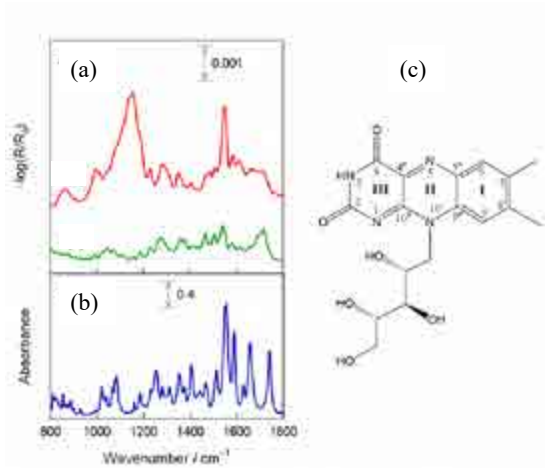
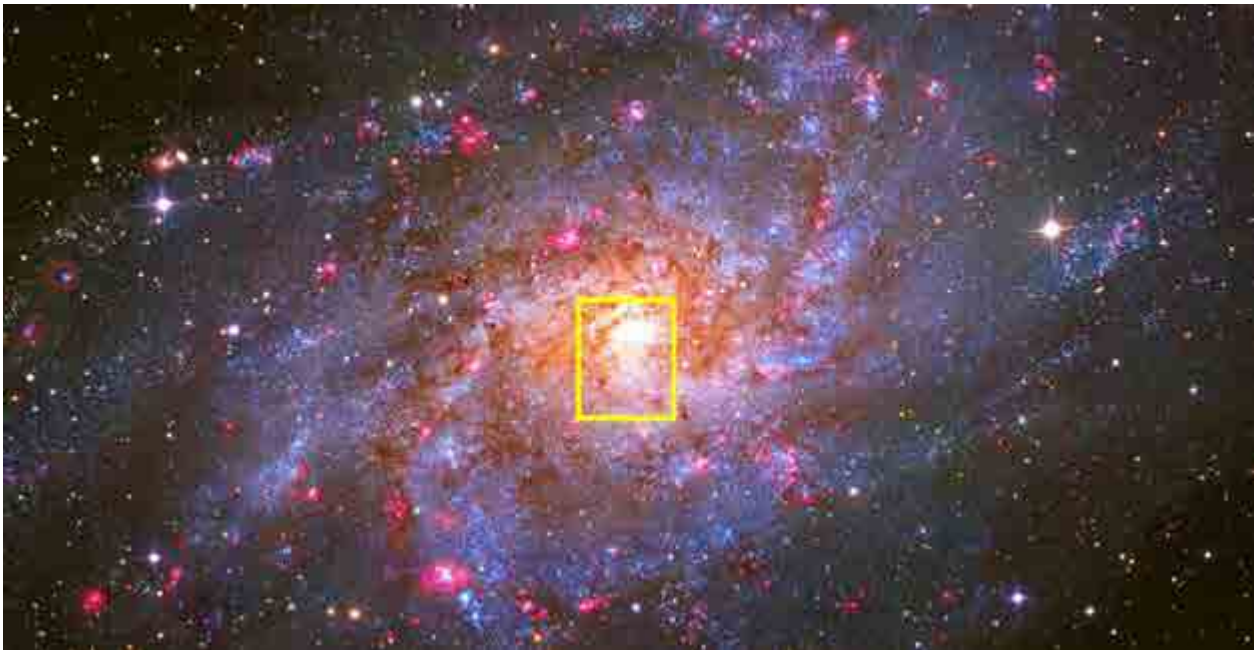


Fig. 2. (a) RAIRS spectra of polymerized riboflavin (red line) and adsorbed riboflavin at the Au electrode (green line). (b) FTIR spectrum of riboflavin in a KBr tablet. (c) Chemical structure of riboflavin.

Astrophysics



Evolution of galaxies

We study complex systems, from star clusters to galaxies, by employing ground- and space-based observations as well as parallel computer simulations of resolved & semi-resolved stellar populations, and active galactic nuclei (AGN).

Spiral galaxy M33

Combined analysis of stellar photometry in the centre of the nearby spiral galaxy M33, performed on the Hubble Space Telescope (HST) WFPC2 images, together with the Herschel Space Observatory (HSO) cold dust emission (160 mm) maps, led to the discovery of a new phenomenon – a tight spatial correlation of young hot main sequence stars (blue) and the reddest stars (red), commonly thought to be old cool red giants. This highlighted the importance of proper accounting for the extreme reddening effects on young stars. Therefore, new 3D dusty models of galaxy evolution are required.

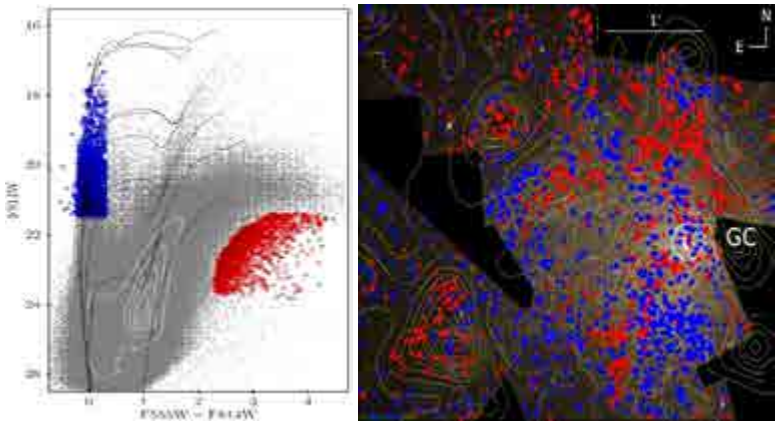
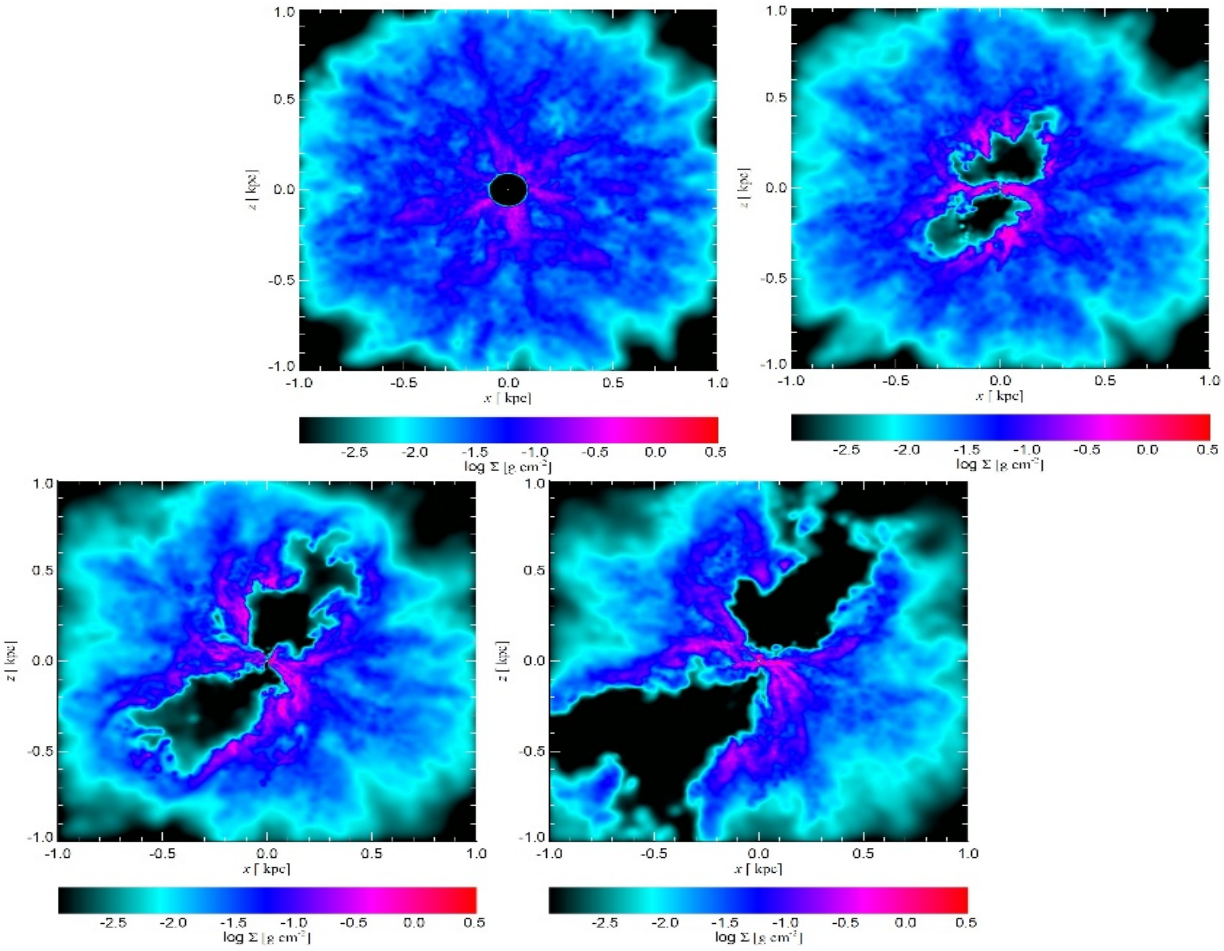


Fig. 1. Subaru (NAO of Japan) image of the M33 galaxy disk (top). The region marked yellow is shown on the HST WFPC2 image (right). Yellow contours show dust emission from the HSO. Stars marked in the CMD blue and red (left) are overploted on the HST image of the M33 center. CMD of the WFPC2 stellar photometry catalog of M33 stars (gray dots) is over-plotted with Padova isochrones (10, 30, 100, 300 Myr, & 3 Gyr, dashed lines). Blue and red dots show young and heavily reddened stars, respectively.



Galactic outflows in AGN

Cosmological models of galaxy evolution usually include effects of feedback by AGN as sub-resolution prescriptions. We showed that the most commonly used prescriptions drastically over-predict the quenching effect that AGN have on their own gas supply, and under-predict the sizes of galactic outflow bubbles. We solved these problems by developing and testing a new prescription for the hybrid SPH/N-body code Gadget-3, which creates outflows with a more realistic size and biconical shape, and allows supermassive black hole feeding simultaneously with the outflow. This new method can be used in cosmological simulations without increasing the computational cost, thus significantly improving the results of galaxy evolution models.

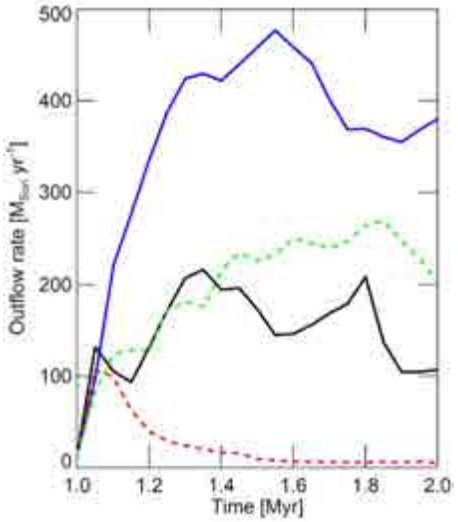


Fig. 2. (above) Progression of AGN outflow. Sequence of density maps showing the growth of a realistic outflow bubble. (below) Mass outflow rates in simulations with different AGN feedback prescriptions (red line – commonly used in cosmological simulations; black & blue – more detailed simulations; green line –our more realistic prescription for cosmological simulations.

Modeling in semiconductors and other materials

Electronic structure calculations of processes at defects in semiconductors

We develop and apply first-principles electronic structure methodologies to describe various properties of point defects in semiconductors and insulators. Most activity is focused in two core areas.

1. Theoretical studies of defects spins in view of their application in quantum information processing and nanometrology. The materials we are currently most interested in are diamond and hexagonal boron nitride. We aim at understanding phenomena such as electron-phonon coupling, optical spin initialization, as well as charge and spin dynamics. This work will help designing the best spin qubits and single-photon emitters.

2. Ab initio theory of radiative and nonradiative processes in connection to energy losses in opto-electronic devices. Recently, our focus is on group-III nitride materials used to make green, blue, and UV light-emitting diodes. Our work has already helped identifying the culprit defects that substantially diminish the performance of these devices.

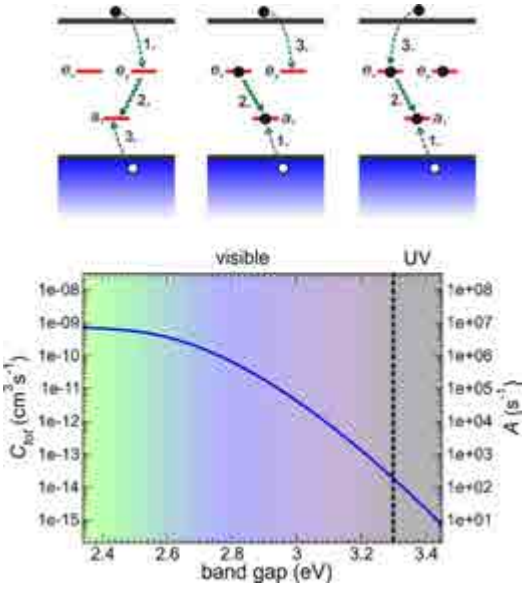


Fig 1. (top) Processes of nonradiative recombination at gallium vacancy complexes in InGaN. (bottom) Calculated nonradiative recombination rates for different band gaps of InGaN alloys.

Plasma oscillations in optically excited GaAs

The oscillations of electron-hole plasma generated by femtosecond optical pulse in freestanding GaAs are studied using Monte Carlo simulations. It is found that following conditions have to be fulfilled in order to observe coherent plasma oscillations:

(i) the intensity of the optical pulse must exceed some threshold value,

(ii) the optical absorption depth must exceed the thickness of the built-in electric field region,

(iii) the generation of electron-hole pairs with uniform illumination is required, i.e., the laser beam with the flattop intensity profile has to be used. The video files of optically excited electron-hole plasma dynamics in GaAs/AlGaAs hetero-structures see in: http://www.sciencedirect.com/science/article/pii/S0030401814000546

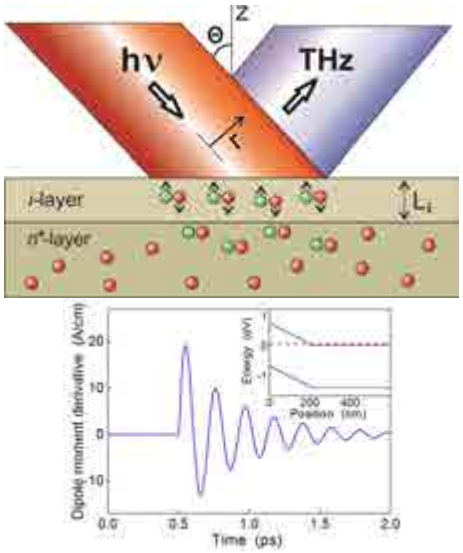


Fig. 2. (a) Schematic representation of excitation of plasma oscillations using femtosecond optical pulse (FOP). The FOP illuminates the semiconductor surface and generates electrons and holes which are accelerated by the built-in electric field. The induced transient photocurrent radiates THz pulse, which travels through some distance in free space and focuses on the detector. (b) Waveforms of temporal derivative of the dipole moment in GaAs structure as obtained from our simulations. The inset shows the equilibrium potential profile, the dashed line indicates the Fermi level.

Free – electron grating and THz generation in GaN MOSFET

The electron transport in MOSFET channel based on 0.02–0.2–0.02 μm n+nn+ wurtzite GaN with the 0.1 μm gate centered in n-region is simulated by Monte Carlo particle technique. It is shown that in channel at positive gate bias the free electron grating in un-gated regions and two electron streams under the gate are formed due to the optical phonon emission. The interaction between these streams results in drain current oscillations up to 5 THz frequency due to the streaming plasma instability.

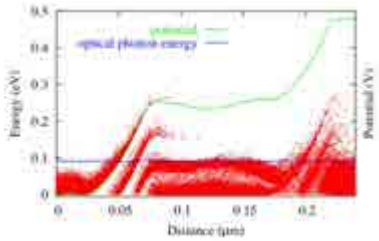


Fig. 3. Instantaneous electron distribution in the energy- coordinate plane (red dots), potential, and optical phonon energy at 0.48 V drain bias at a temperature of 80 K in MOSFET channel. Two electron streams are seen under the gate: just under optical phonon energy and in low energy region.

Wave fronts in metamaterials

Graphene is still of interest, mainly due to the relativistic behavior of its electrons and holes. A nice example is the Klein effect when the electron penetrates the electric barrier (a) converting itself into a hole. In this case the hole demonstrates the behavior similar to that of the wave in metamaterial as it's phase and group velocities are of opposite sign. In spite of the negative phase velocity in the barrier, the front of electronic wave continues it's non-perturbed motion (b). Such a behavior differs essentially from the propagation of the electromagnetic wave in the transmission metaline composed of lump element cells (c) when the opposite sign of above velocities take place in the finite frequency region. In the contour plot (d) the three different velocities are clearly seen. The comparison of the two wave front propagations indicates the essential sensitivity of fronts to the details of dispersion relation in metamaterial.

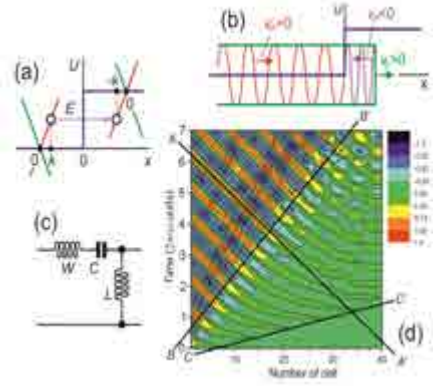


Fig. 4. (a) The barrier and electron spectrum in graphene, (b) front penetration into the barrier, (c) the unit cell of the transmission metaline with lumped elements, (d) contour plot of the front propagation in the transmission metaline, solid lines correspond to: AA' - negative phase velocity, BB' - positive group velocity, CC' - velocity of fast precursor.

Phase transitions in metal-organic frameworks

A combined experimental and Monte Carlo study is proposed to describe an order–disorder structural phase transition in perovskite-based $[(CH_3)_2NH_2][M(HCOO)_3]$ (M = Zn^{2+}, Mn^{2+}, Fe^{2+}, Co^{2+} and Ni^{2+}) metal–organic frameworks (MOFs). The model is constructed on a simple cubic lattice where each lattice point can be occupied by a $(CH_3)2NH_2^+$ (DMA^+) cation in one of the available states. The main interaction is the nearest-neighbor Potts-type interaction (e_p), which effectively accounts for the H-bonding between DMA^+ cations and $M(HCOO)_3$ cages. The model is modified by accounting for the dipolar interactions (e_{dd}) which are evaluated for the real monoclinic lattice using density functional theory. The obtained results indicate that the three-state Potts model correctly describes the phase transition order in these MOFs, while dipolar interactions are necessary to obtain better agreement with the experimentally measured polarization. We show that in our model with substantial dipolar interactions the ground state changes from uniform to the layers with alternating polarization directions (Fig. 5).

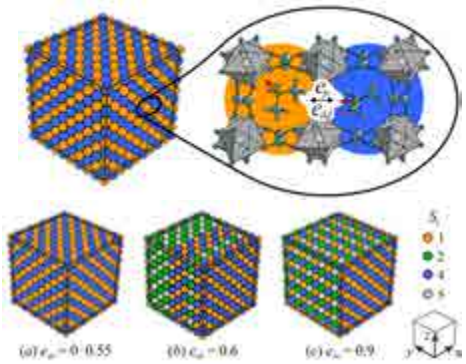
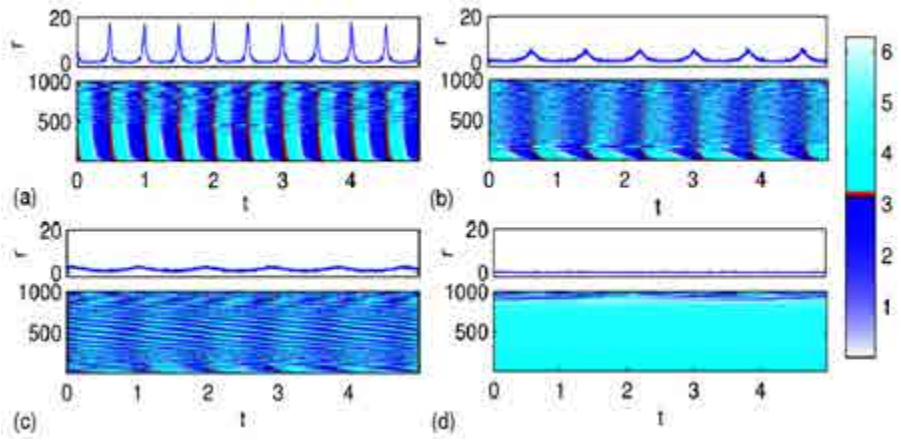


Fig. 5. (top) Correspondence between color coding, structure and cation states (polarization directions). (bottom) Orderings at low temperature obtained for different dipolar interactions: (a) 0–0.55 (uniform structure), (b) 0.6 (a typical layered structure) and (c) 0.9 (interpenetrating monolayers). Color coding is used to differentiate between different cation states.



Dynamics of the firing rate (top graphics in each panel) and the phases presented by colors (bottom graphics in each panel) of N = 1000 synaptically coupled quadratic integrate-and-fire neurons.

Synchronization phenomena in complex oscillatory networks: reduction of microscopic system to a low-dimensional system of equations

Complex systems composed of a large number of interacting nonlinear dynamical elements are ubiquitous in nature. Synchronization and other collective effects in such systems is a pervasive topic in physics, chemistry, biology, and social networks. The synchronization of oscillations is a mechanism for neural communication, which endows individual brain areas with the ability to perform specific tasks. Conversely, extremely strong synchronization may cause various neurological disorders. To better understand the synchronization phenomena in complex neural networks, one can consider the problem in the thermodynamic limit of infinity number of interacting neurons. In certain cases such an approach allows a reduction of the microscopic equations to a low-dimensional system that defines the dynamics of the macroscopic system parameters.

We have analyzed the dynamics of a large network of coupled quadratic integrate-and-fire neurons (QIF), which represent the canonical model for class I neurons near the spiking threshold. The network is heterogeneous, since it includes both inherently spiking and excitable neurons. The coupling is global via synapses that take into account the finite width of synaptic pulses. Using a recently developed reduction method based on the Lorentzian ansatz, we have derived a closed system of equations for the neuron's firing rate and the mean membrane potential, which are exact in the infinite-size limit. The bifurcation analysis of the reduced equations reveals a rich scenario of asymptotic behavior, the most interesting of which is the macroscopic limit-cycle oscillations. We have shown that the finite width of synaptic pulses is a necessary condition for the existence of such oscillations. The robustness of the oscillations against aging damage, which transforms spiking neurons into non-spiking neurons, have been analyzed. The validity of the reduced equations have been confirmed by comparing their solutions with the solutions of microscopic equations for the finite-size networks.

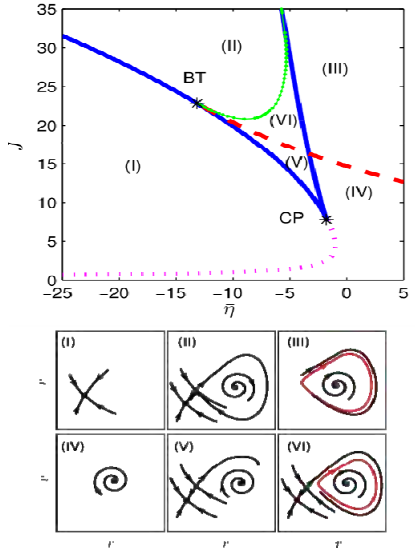


Fig. 1. (top) Two-parameter bifurcation diagram of the macroscopic QIF neuron model. (bottom) Typical phase portraits of the system corresponding to different regions of the parameters marked in the top panel by Roman numerals.

Metrology

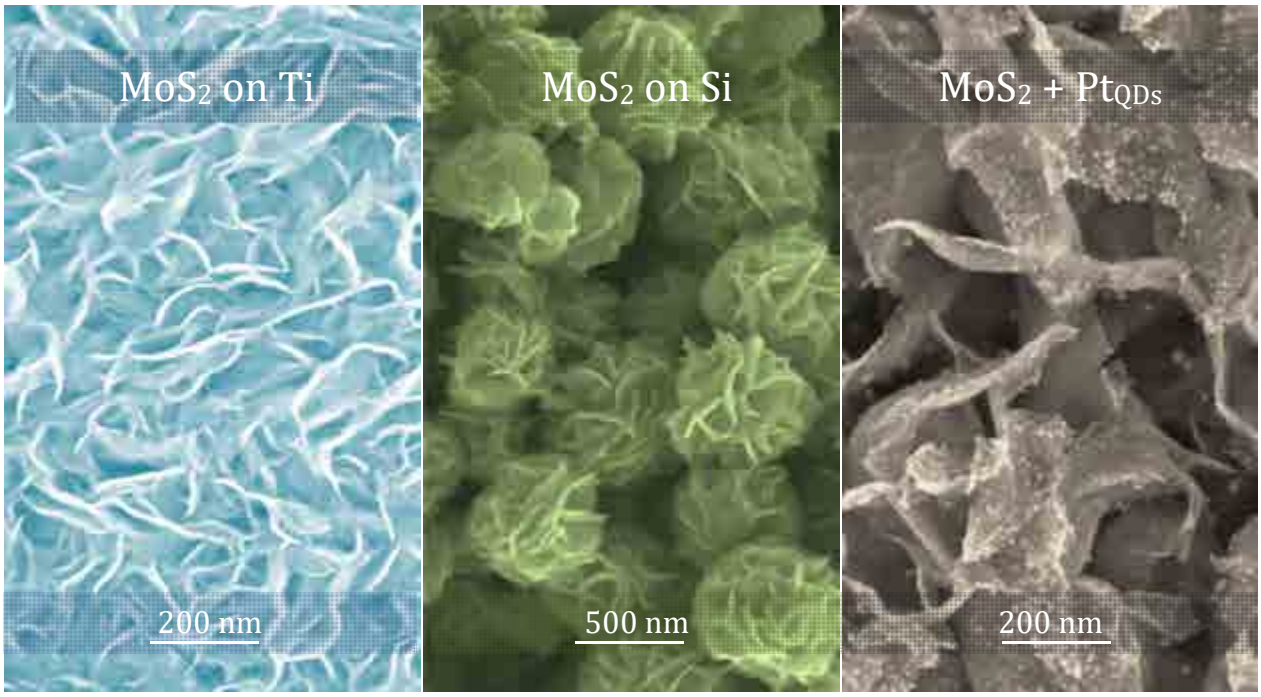
Research in National metrology institute of Lithuania

Man's knowledge of nature, the universe, and how to adapt nature to his purpose, advances in step with his ability to measure precisely.

The metrology assures the correctness, accuracy and reliability of measurement results. The measurement as such is not the specificity of the metrology science. The core of metrology lies in validation of the result, particularly by specifying its actual limitations. Since July 1, 2014 the Metrology Department was authorized to perform and implement the functions of the National Metrology Institute.

The Metrology Department maintains national standards in five different metrology fields. The **Time and Frequency Standard Laboratory** is reproducing the value of a unit of time (the second) and the unit of frequency (the Hertz). Its mission is the representation of Lithuanian Coordinated Universal Time UTC(LT), in this way ensuring the traceability of the magnitudes reproduced to the International System of Units (SI), disseminating them to Lithuanian scientific establishments, personal and legal bodies by calibrating their working standards and measurement devices, disseminating Lithuanian time scale, and other relevant means. The mission of the **Electrical Standards Laboratory** is maintaining and developing the standards of unit of voltage (the Volt) and unit of resistance (the Ohm), thus ensuring their traceability to the SI system, calibrating working standards and measurement devices, pursuing research in the field of measurement of voltage, resistance and electrical current. The **Temperature Unit Standard Laboratory** is implementing the international temperature scale ITS-90 and the value of the unit of temperature (the Kelvin), and ensuring their traceability to the SI system. Lithuanian national standard of the temperature unit in the range from -195°C to +961,78 °C is of the primary level and +1084,62 °C freezing point of Cu is of the secondary level. In the **Ionizing Radiation Metrology Laboratory** radionuclides have been standardized by applying primary methods. The Triple-to-Double Coincidence Ratio method was used for standardization of tritium achieving the expanded uncertainty of the activity <1%. The response of dose calibrators was compared with the secondary standard of the National Metrology Institute in Prague for measuring activities of short-lived radionuclides used in nuclear medicine: F-18, Ga-67, Tc-99m, In-111, I-123, and I-131. The metrological activity is not restricted to standards of the physical units. Reliable and accurate chemical measurements in health care, food safety and environment protection fields are provided by the **Laboratory for Metrology in Chemistry.**

Electrochemistry & tribology



Electrochemical materials science

The R&D activities in this area are focused on the development of new functional materials, such as alloys of light and refractory metals (Mg, Al and Cr, Nb, Zr, Ta), nanomaterials and their arrays, including semiconductor nanowires loaded inside the alumina pores and nanostructured titanium or iron oxides, transparent conductive oxide layers and their heterostructures, corrosion resistant nanostructured electrodeposits of Cr and Zn alloys, etc.

Much effort is also devoted to the search of **new methods for** the synthesis of superparamagnetic and luminescent nanoparticle and investigation of their application possibilities in nanomedicine; **new effective materials** for photovoltaic and nanoelectronic technologies; **technologies** of deposition of smart coatings with active corrosion protection ability for metals in aggressive environments.

Electrochemical and chemical (electroless) as well as physical (magnetron sputtering, atomic layer deposition) methods are applied for the surface modification and production of new functional materials with exceptional anticorrosive, electrocatalytic, magnetic, mechanical or other properties. The integral part of the process of new materials development is thorough characterization of their structure, morphology, chemical composition as well as investigation of their corrosion behavior in solutions (including simulated biological ones) and atmosphere. Environmental friendliness is an imperative for all newly developed technologies. Another trend of scientific research is related to tribology and formation of compositions of biofuels, lubricants and plasticizers, using biodegradable components. These activities include search for tribologically efficient materials for new type anodic aluminum coatings with exceptional resistance to friction and attrition. The results are tested directly in Anodization pilot plant, located in the Chemical technologies department of the Center. Corrosion, tribological, physical and electrochemical studies on the interaction of biofuels (ethanol, biodiesel, biolubricants) with metal surfaces are carried out as well.

Corrosion Testing Laboratory, accredited in 2007, performs corrosion testing and evaluation of the corrosion-caused changes of metals, alloys, composite coatings, paints and lacquers in natural and artificial atmosphere as well as testing of microbially induced corrosion of materials in atmosphere and model medium.

Electrochemical formation of nanotubed alumina-graphene composite films

The formation of novel alumina-graphene composite films with a novel design (Fig. 1), unprecedentedly low optical gap (1.53 eV) and exciting chemical inertness has been developed in 2016 by Nanostructures laboratory group via Al anodizing in tartaric acid solution at extremely high current densities exceeding burning initiation. These properties were ascribed to entrapping of significant amount of graphene-based materials at the top- and back-side of the film.

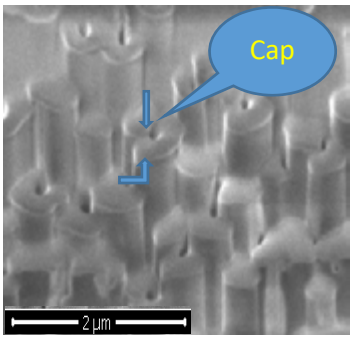


Fig. 1. Panoramic FESEM images of alumina film formed by Al anodizing in aqueous solution of 0.8 M tartaric acid at 40 A dm^{-2}.

Towards efficient solar water splitting

Researchers of Metals Electrochemistry Laboratory have employed "solar cell + electrolyzer" strategy in a case study of water splitting using a simple n-Si/Ni Schottky solar cell connected to water electrolysis cell with the most efficient water splitting electrodes. The role of hydrogen peroxide formation as an intermediate in oxygen evolution reaction (OER) has been newly revealed and explains why an oxygen evolution is not taking place at the thermodynamically expected 1.23 V potential. Oxidation of water to intermediate peroxide state (with $E^0 = 1.77$ V) has been shown to be the threshold step in OER. It has been demonstrated that separation of the processes of solar harvesting and electrolysis avoids photo-electrode corrosion, utilizes optimal electrodes for hydrogen and oxygen evolution reactions and the pursued ~10 % efficiency in solar-to-hydrogen conversion is achievable with a standard 18 % efficient household roof Si-solar cells. Strategy to increase efficiency above 15 % for a single junction cell has been outlined.

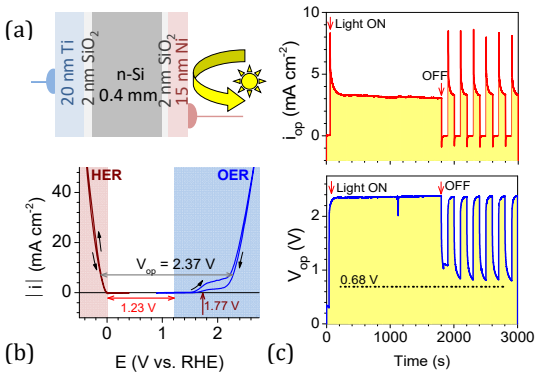


Fig. 2. (a) Scheme of n-Si/Ni solar cell. (b) Voltammograms of Pt cathode and Ti/(Ir+Ta) oxide anode. (c) Illumination dependent variation of photocurrent and voltage in water electrolysis cell.

Tribology-based recycling of waste rubber into devulcanized powder

End-of-Life Tires (ELT) present major problems in environment, transport, agriculture and elsewhere, so innovative methods to recycle waste rubber are highly welcome. In collaboration with UAB Gumos technologijos and Nizor Ltd. (Israel) within Eureka! Programme, last year researchers from FTMC Tribology Laboratory completed a project E!9962 "OzoRubber", where they developed a new process to recycle rubber waste. Rubber crumbs, e.g. ground ELT, were mixed with selected chemicals and exposed to high shear between moving surfaces. As a result, rubber was ground into powder and partially devulcanized along with dramatically increased roughness (Fig. 3). Devulcanized rubber powder can be used to formulate new rubber compounds at 70% or higher treat rates, as shown by "OzoRubber" partners. Several prototypes have already been developed for tire manufacturers and construction industry. Research continues to further improve the devulcanizing agent composition.

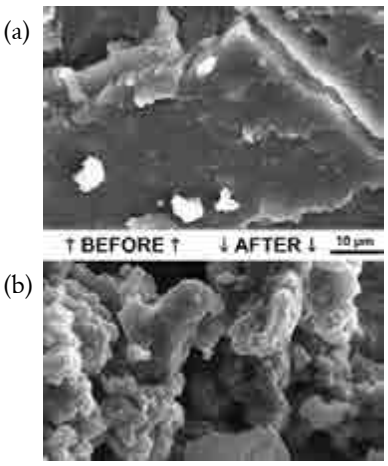
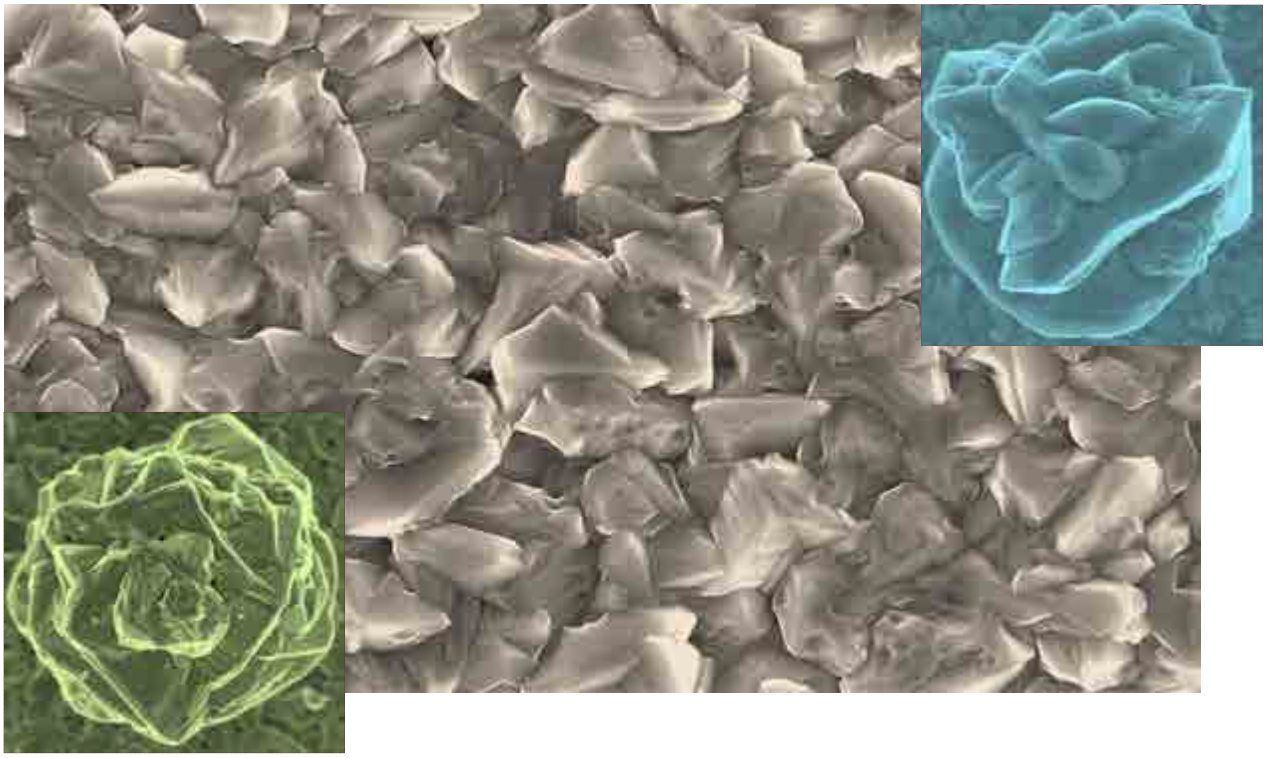


Fig. 3. SEM of (a) old tire rubber and (b) development of highly porous surface due to tribological processing.

Materials for catalysis



Electroless metal deposition: from fundamental research to application for microelectronics, fuel cells and in other areas

Electroless metal plating is well-known method for deposition of metal coatings by a controlled chemical reduction and formation of small (nano-scale) metal particles. The R&D activities of the Department of Catalysis in this field are focused on the development of new electroless metal plating processes as well as fundamental studies of reactions occurring in autocatalytic metal ions reduction by means of electrochemical quartz crystal microgravimetry. The Department of Catalysis for LAM Research corporation (USA) developed following electroless deposition technologies: (i) of continuous Pt and Pd layer using complexed Co^{2+} metal ion as reducing agent, (ii) of continuous Co and Ni layers using complexed Ti^{3+} metal ions as reducing agent, (iii) of continuous Pd layer using complexed Co^{2+} metal ions or Ti^{3+} metal ions as reducing agents. Also, developed the technologies for deposition of high surface roughness copper coatings by electroless plating and thick (>20μm) electroless Cu coatings used as contacts in solar cells. The latter has been introduced in industrial solar cell laboratory in UAB „Precizika-MET SC“. The electroless metal plating method is also successfully used for fabrication of new catalytic materials for fuel cells. The non-noble metal and noble metal catalysts with low amount of noble metal supported titanium or titania nanotube arrayed surfaces, carbon, graphene powder or other supports with enhanced activity towards the oxidation of various fuels has also been developed. The catalysts obtained are promising anode materials and can be used in fuel cells.

Development of catalysts for fuel cells

Simple and cost-effective electrochemical and chemical methods have been developed for preparation of an efficient cobalt catalyst with a fiber structure and decorated with Au or Pt nanoparticles (Fig. 1a,b). Cobalt coating with a fiber structure and the thickness of ~3 mm (Co_{fiber}/Cu) was electroplated on the copper surface. Au or Pt crystallites were deposited on the Co_{fiber}/Cu surface via the galvanic displacement technique. The fiber structure cobalt decorated with Au or Pt nanoparticles was found to demonstrate enhanced catalytic activity towards the hydrolysis of sodium borohydride, as compared to that of Co_{fiber}/Cu, as well as towards oxidation of sodium borohydride, hydrazine and methanol in an alkaline medium.

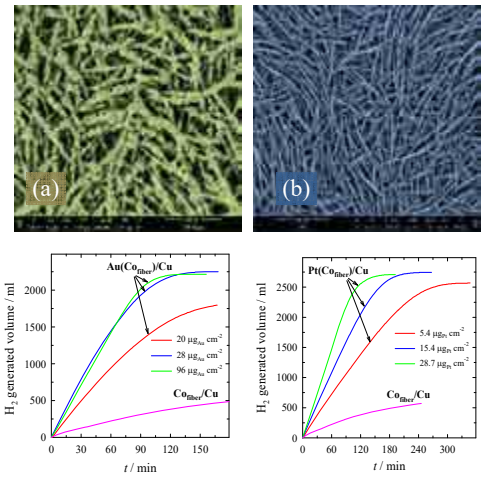


Fig. 1. SEM views of Au/Co_{fiber} (a) and Pt/Co_{fiber} (b) and corresponding curves of H_2 generation from 5 w% $NaBH_4$ + 0.4 w% NaOH solution catalyzed by the same catalysts.

Development of catalysts for nano and micro spacecraft thrusters

RJS "NanoAvionics", in colaboration with the Department of Catalysis, developed the prototype of the small satellite thruster (Fig. 2a). A novel solid state catalyst bed for nano and micro spacecraft thrusters has been designed (Fig. 2b). Best results for the propulsion system were obtained using the nickel foam (Fig. 2c) plated with the platinum and rhodium (Fig. 2 d,e).

The prototype of the small satellite thruster will be launched into the space and tested under real conditions in the spring of 2017.

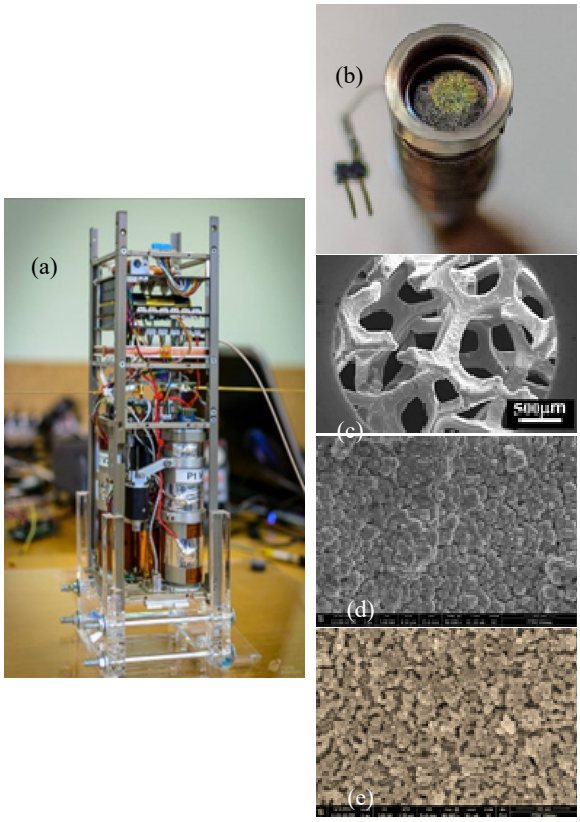
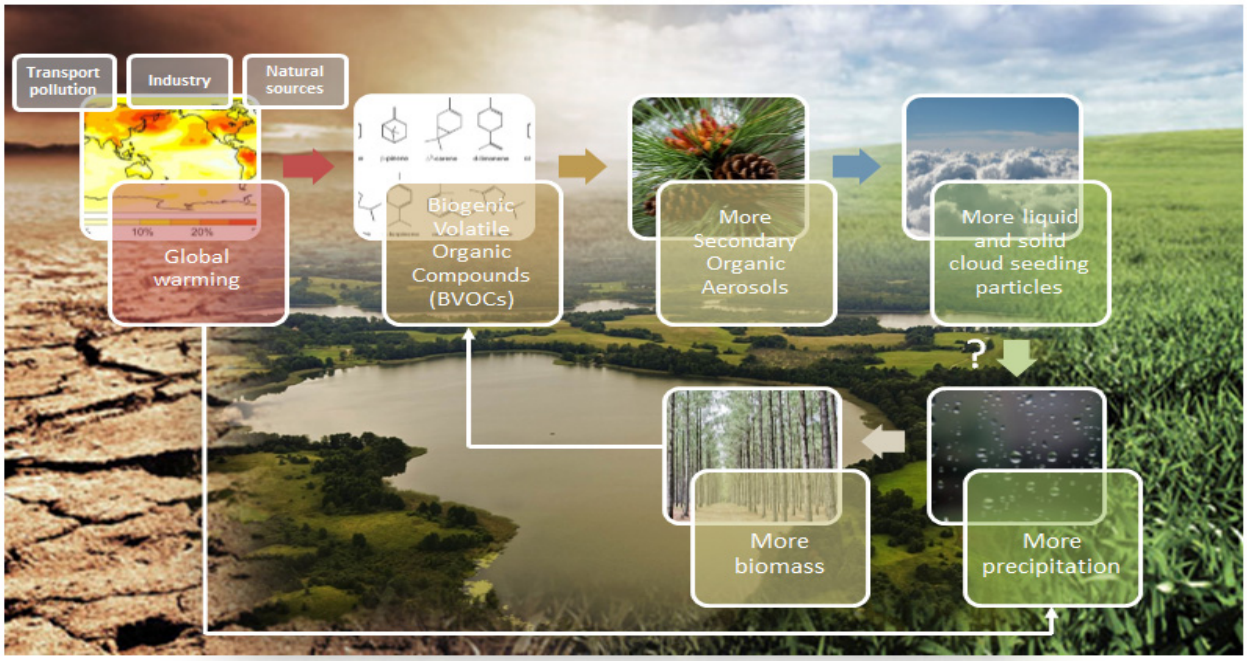


Fig. 2. (a) The prototype of the small satellite thruster. (b) The prototype of created catalyst for the small satellite. SEM views of the Ni foam (c), Pt (d) and Rh (e) deposited on the Ni foam surface.

Environment



The environment-friendly technologies for observation, simulation, prevention and mitigation of atmospheric pollution, and relation to the climate change

A modern environmental research relies on solutions that bring together the recent achievements in technologies and sciences that underpin our understanding of the Nature to deliver a sustainable environmental future and economic growth. In the Department of Environmental Research the main focus is directed towards investigations of chemical composition of non-refractory submicron aerosol particles using mass-spectrometry methods as well as to processes that control aerosol formation and evolution. We are also interested in the impact of changing atmospheric composition on air quality, human health, climate change and ecosystems. By conducting the fundamental and applied research, we are trying to find long-term solutions, especially in experimental techniques devoted to aerosol studies, with the ultimate goal of promoting development towards modern environmentally-friendly technologies based on radionuclide methods which are suitable in the environmental science technologies in general and may be applied in the vicinity of facilities in particular.

Objectives: To develop and improve principles, means and technologies of the environment quality evaluation and to ensure the scientific competence in the fields of environment physics and chemistry, environment contamination and climate changes.

Tasks:

i) Development of technologies and equipment for the environment protection quality control as well as methods and experimental basis in the environmental research, investigation of micro-admixture dynamics and balance in the environment components as well as characterization of the impact of environment contamination on climate change.

ii) Evaluation of efficient instrumentation and assessment of methods suitable for characterization of the impact of industry, transport and consumer sectors on the environment quality. The Department is especially interested in combining of spectrometric methods in evaluating the aerosol particle mass and sizes as well as in investigations of physical-chemical aspects of the aerosol particle formation.

Development and application of innovative techniques for atmospheric organic aerosol measurement

Fossil and non-fossil source contributions to atmospheric carbonaceous aerosols

Separation between fossil and non-fossil primary and secondary contributions was obtained by coupling Aerosol Chemical Speciation Monitor *Positive Matrix Factorization* results and elemental (EC) and organic (OC) carbon fractions. Carbonaceous aerosol was described to be composed of the following four categories: fossil OC_f and EC_f, attributed to primary and secondary fossil fuel combustion, and non-fossil OC_{nf} and EC_{nf} attributed to primary and secondary biomass burning (BB), cooking and biogenic emissions (Fig. 1). The OC_{nf} was found to be the dominant fraction of the atmospheric submicron particulate matter PM_1, with the primary (POC_{nf}) and secondary (SOC_{nf}) fractions contributing to the total carbon (TC) by 26–44% and 13–23%, respectively. The 5–8% of the TC had a primary fossil origin (POC_f), whereas the contribution of fossil SOC_f was 4–13 %. The data for EC_{nf} and EC_f were 13–24% and 7–13%, respectively.

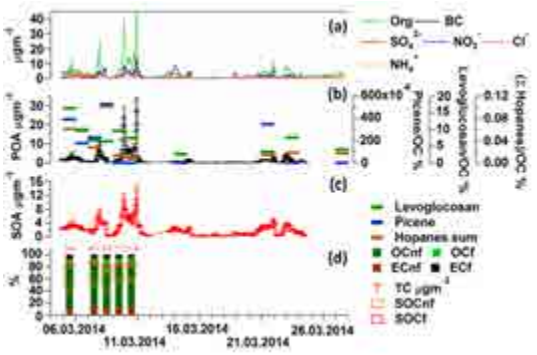


Fig. 1. Average chemical composition and time series of organic aerosol (OA) (µg·m^{-3}): (a), (b) time series of the POA factor and percent contribution of the corresponding tracer species to total OA, (c) time series of the SOA factor, (d) relative source apportionment of TC during the BB event.

Researching the mechanism of the new particle formation in the atmosphere

The seasonal variations of the particle number concentration (PNC) of nucleation (8.7–20 nm), the Aitken (20–100 nm) and accumulation modes (100–840 nm) were estimated to classify particle formation and growth rates. The input of the nucleation mode to total PNC was shown to be limited by the inputs of Aitken and accumulation modes. It was determined that those limits are the same for new particle formation (NPF) event days and non-event days (Fig. 2). Determined empirical equations allowed developing a simulation model of the particle size distribution dynamics in the atmosphere.

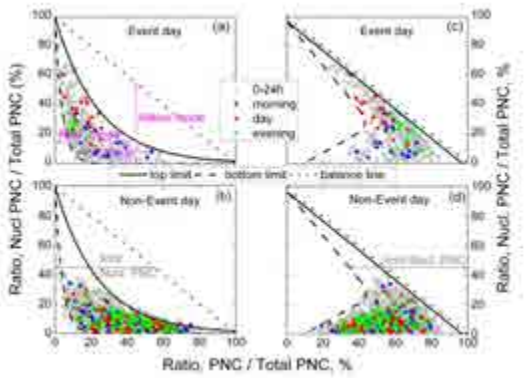


Fig. 2. Dependences of the nucleation mode PNC on the accumulation and Aitken mode PNC.

Nuclear

Nuclear research: applications today and innovative technologies and methods in future

The Department of Nuclear Research develops and applies known and innovative technologies and methods in nuclear spectroscopy, nuclear energy safety, radiation protection, radiochemistry, radioecology, mass spectroscopy, Mössbauer spectroscopy, ion beam analysis and modification of materials. The keystones of the safety field are the safe operation assurance of nuclear facilities, the optimization of radioactive waste management, the assessment of shielding materials and the comprehension of processes of radionuclides transport through engineering barriers to enable nuclear facility safety. Special attention is paid to environmental impact assessment of energy generating facilities, elemental and isotopic analysis of groundwater, soil, lake silt, food fabrics and products, and also industrial stocks and medical samples with sensitivity up to 1 ppq (for non-interfered isotopes). Application of stable isotope ratio analysis ($\delta^{13}C$, $\delta^{15}N$, $\delta^{18}O$ and $\delta^{34}S$) in environmental, biomedical and food samples stimulates new promising technologies. Measurements of stable isotopes in marine aerosol allow analyzing the climate-aerosol-cloud feedback systems: revealing of dual carbon pools contributing to fractional organic matter enrichment leads to reassertion of the hypothesis that organic matter enrichment in sea-spray is directly linked to primary production. The ^{14}C measurements open the potentially new field of activity related to carbon dating and analysis of triple carbon ratio of dedicated samples. Complimentary information on material properties (magnetic properties, oxidation and corrosion of iron compounds) is determined by Mössbauer spectroscopy. Development of ion beam methods for material analysis and modification is important part of our activities having intersection both with semiconductor materials and applications for laser technology. Investigation of polyethylene 2,6-naphthalate scintillator films opens new possibilities for application of simple scintillator material for detection and spectroscopy of ionizing radiation particles.

Advanced technologies for radioactive waste characterization

The experimentally validated model (using MCNP, SCALE program packages) is developed for precise evaluation of the neutron induced activity in any position of the 3D RBMK-1500 reactor core constructions. The real distribution of radionuclides and processes of radionuclides transport are investigated using nuclear spectroscopy, radiochemistry and methods of structural analysis (SEM, RS, XPS). Identification of the most significant radionuclides in irradiated graphite and prediction of the radiation dose rate for the personnel handling with irradiated graphite waste at Ignalina NPP Unit 1 have been accomplished.

Safety technologies for spent nuclear fuel (SNF) storage in CONSTOR® RBMK-1500/M2 cask and, in particular, the impact of RBMK-1500 burn-up credit on effective neutron multiplication factor were studied using pre-generated ORIGEN-ARP spent nuclear fuel composition libraries. Burn-up credit application in criticality analysis of SNF reduces conservatism of usually used fresh fuel assumption and implies positive economic impact for SNF storage. The obtained results are important for further decommissioning of the Ignalina nuclear power plant and other RBMK type reactors.

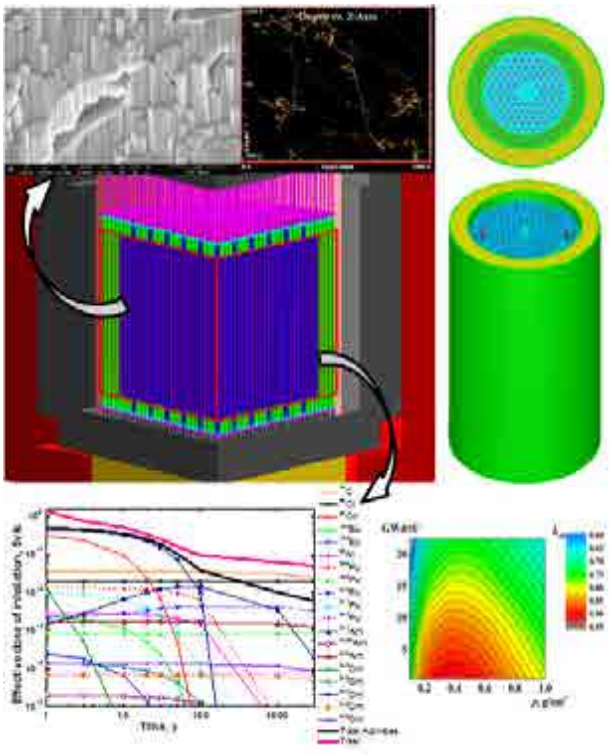


Fig. 1. Morphological analysis of RBMK graphite: magnified view of graphite and DPA rate vs distance in the graphite;
3D model of ¼ of RBMK reactor core and effective inhalation dose for the personnel handling with irradiated graphite; CONSTOR® RBMK-1500/M2 cask: keff inside SNF cask as a function of burn-up and water density for 2.8% enrichment fuel.

Ionizing radiation detection

using industry grade polyethylene 2,6-naphthalate (PEN) scintillator films. These films were investigated as scintillator material for detection and spectroscopy of ionizing radiation particles. A wide range of particles, such as alpha, beta, gamma particles, protons and neutrons, were detected and spectra were measured using PEN scintillation. The energy deposition in the samples was calculated by Monte Carlo computer modeling. Separate neutron/gamma and alpha/beta pulse shapes were obtained, using pulse shape discrimination. The figure of merit was used to determine the quality of discrimination of particles.

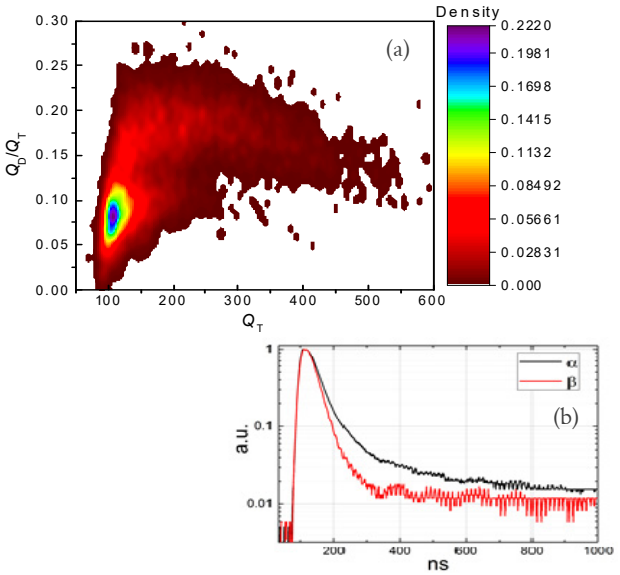


Fig. 2. (a) Separation of neutron and gamma pulses using PEN.
(b) Alpha and beta particles detection.

Mass spectrometry for new applications

The isotope ratios exhibited a strong correlation with the fractional organic matter (OM) enrichment in sea spray aerosol. A model comprising two organic matter pools is proposed to explain the observations in a manner consistent with the main biogeochemical processes. This model is harmonious with the preferential enrichment of fresh colloidal and nano-gel lipid-like particulate matter in sea spray particles and the observed depleted $\delta^{13}C$ ratio resulting from isotope equilibrium fractionation coupled with enhanced plankton photosynthesis in cold water (−2°C to +8°C). The results reassert the hypothesis that OM enrichment in sea-spray is directly linked to primary production and, consequently, can have implications for climate-aerosol-cloud feedback systems (Fig. 3).

Stable isotope analysis was applied to describe the poultry house environment. The analysed examples imply that stable isotope analysis can be used to examine the indoor environment along with its biology and ecology and serve as an informative bioanalytical tool.

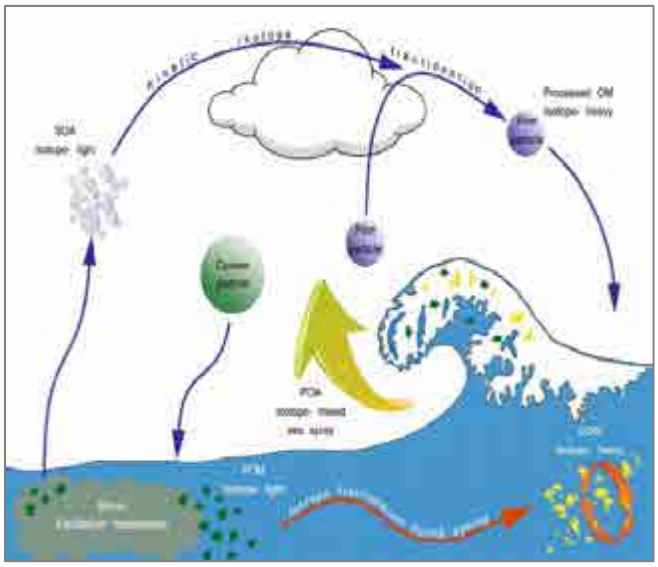


Fig. 3. Marine organic matter cycling corroborated by a proposed model.

Tandetron 4110A ion accelerator

is used for structural characterization of advanced optical coatings. The prototype of $In_xGa_{1-x}As/GaAs$ – based semiconductor saturable absorber mirrors (SESAM), used for passive mode-locking at wavelengths of around 1064 nm of the Yb-doped fiber lasers, were manufactured at high temperature using MBE growth and subsequent ion implantation using Tandetron 4110A and annealing. The post-growth processing techniques of implantation and annealing provide a possibility to tune absorber recovery speed to a desired value (from several hundred to few picoseconds) with a reasonable accompanied drop in modulation depth and increase of saturation fluences allowing SESAM for operation far below the damage threshold. Valuable information on technology of complex structures for laser beam applications was obtained. It helps to control various stages of sputtering process and understand the effects of additional element or layer implementation on the final refractive index distribution of coatings and their resistance to laser radiation.

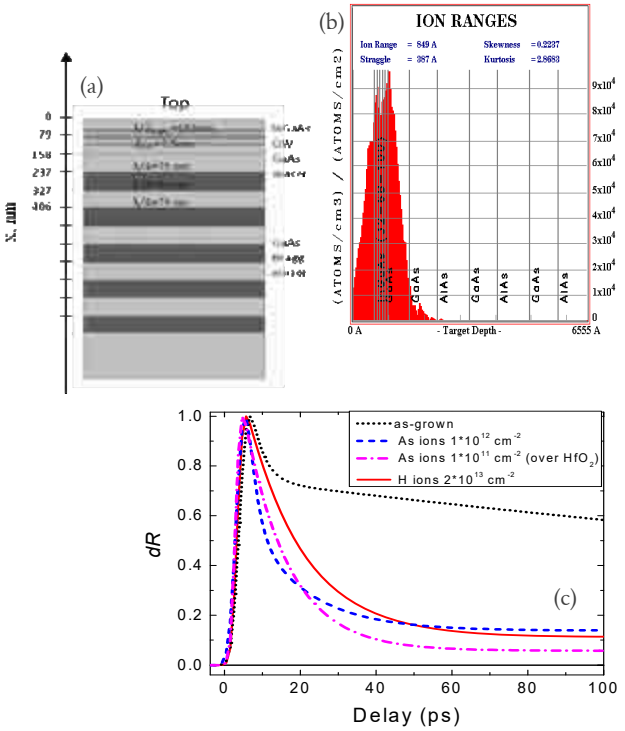
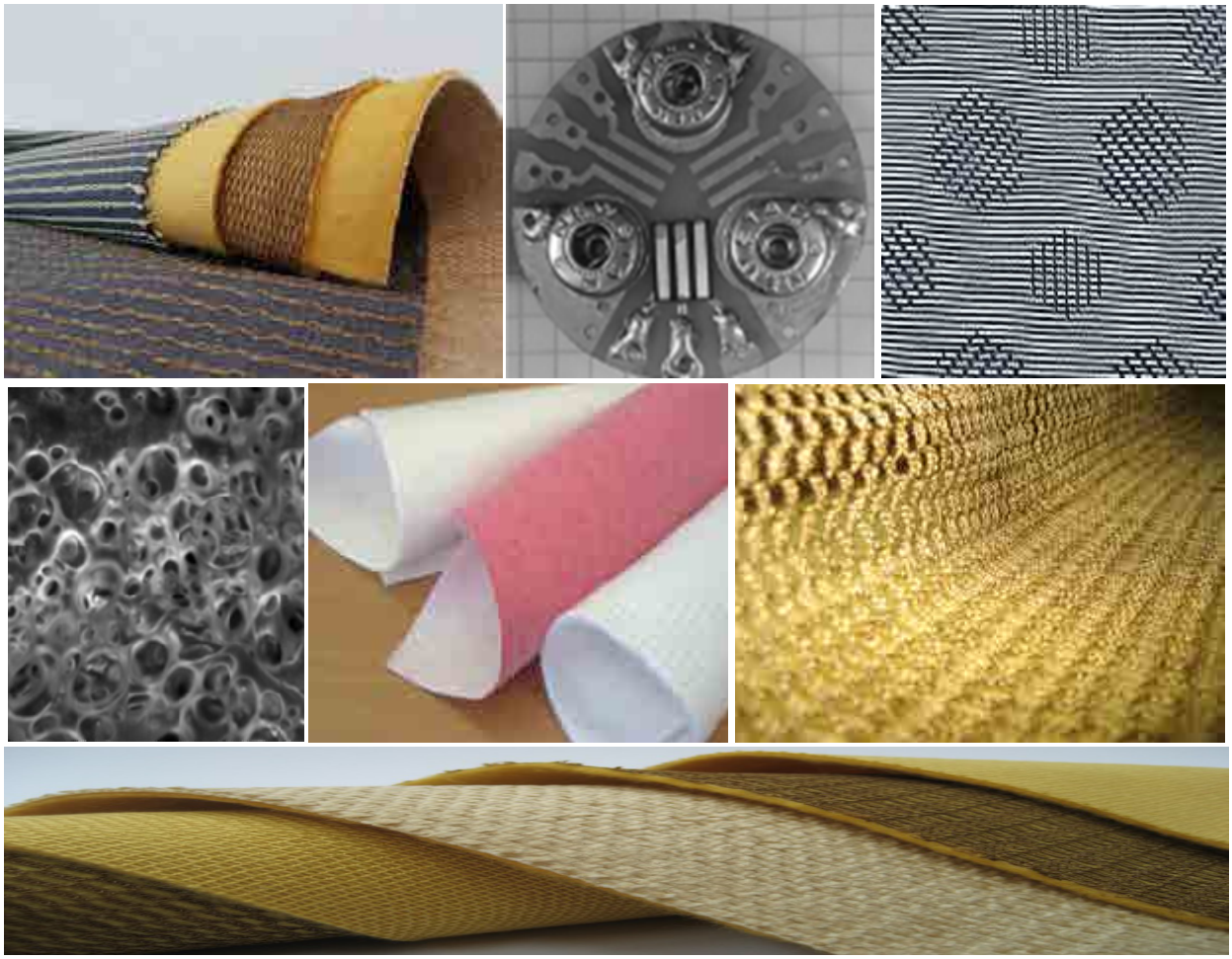


Fig. 4. (a) Antiresonant structure of SESAM without HfO_2 layer. (b) The 10keV H^- ions distribution in antiresonant SESAM. (c) Time-dependent differential reflectivity *dR* at 1064 nm after implantation of various ions and annealing.

Textile technologies



Advanced textile materials

Multidisciplinary research opens new opportunities for the development of textile technologies, tailor-made solutions and products for high value applications. The results of the multidisciplinary research can help the textile not only to ensure and support human well-being for leisure, active lifestyle and safety, but also make the applied textile friendlier for the surrounding environment. This can be achieved by combining a wide range of technological advances in such areas as information technology, mechatronics, robotics, advanced materials, bio– and nano– technologies. The research in Textile Institute is mainly focused on textile materials with (multi)functional properties processed by plasma-chemical surface treatment, coating technologies and micro - and nano – finishing. By using bio-ceramics, we develop smart textile garments with active thermoregulation function and phase change materials. Also, garments with wearable electronics and smart heating T – shirts produced as prototypes. We perform numerical modelling of the heat exchange in textile garments as well.

Textile institute offers a wide range of services:

- testing of textile materials in accredited laboratory and certification of protective clothing at notified body,
- examination of quality of textile materials,
- prototyping of woven and knitted fabrics and garments and applied research for industry.

Textile institute is a place of fresh ideas, innovative minds and successful solutions.

Development of materials with thermoregulatory properties

The heat power, which is detectable by a human body, is most efficiently transferred by the far infrared radiation. We investigated infrared radiation (IR) textiles as an innovative brand of functional textiles that have presumptive health and well-being functionality. Bio – ceramic additives (BCAs) were used as absorbers and emitters of IR radiation. It was found that even small amounts of BCAs can change the overall IR attenuation coefficient of the fabric. The BCAs were introduced directly into the fabric by impregnating, printing and full area coating. The heat resistance of fabrics enhanced by additives, the three dimensional (3D) warp knitted fabric, in particular, was investigated theoretically and experimentally to determine the influence of the modification to the IR absorption. Samples of 3D knits have been produced, in which the outer and connecting layers were made of polyethylene terephthalate (PET) yarn and Ti, Ge, Al, Si elements containing additives able to accumulate infrared radiation flux. Different finishing methods, such as padding, exhaust and printing, were investigated in order to determine proper concentrations of BCAs.

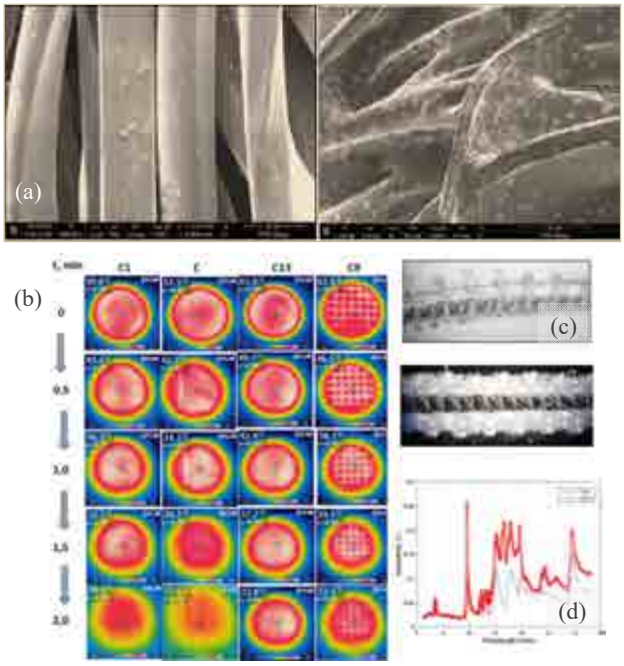


Fig. 1. (a) SEM micrographs of fabrics with $TiFe_2O_5$ or $CoTiO_5$ additives.
(b) Thermal signatures of heat retention dynamics in textiles.
(c) Structure of 3D textiles.
(d) Measured values of absorptivity of pure knit and knit with BCAs.

Development of smart heating textile

The garment with smart heating system was developed. The silver-plated polyester yarns were used to provide electrical conductivity for the knitted structure. The micro-controller with a heating dynamic data storage function was programmed and produced for controlling operations of two heating elements. The prototype of T-shirts with two heating elements placed on the back side of the garment was produced. The heating elements were isolated from potential exposure to moisture. The field tests of the developed model were carried out in different climate conditions, and acceptable values of temperature of both heating elements were fixed. The continuous operating time was determined. It was demonstrated that the developed heating system can provide a comfort micro-climate to the user.

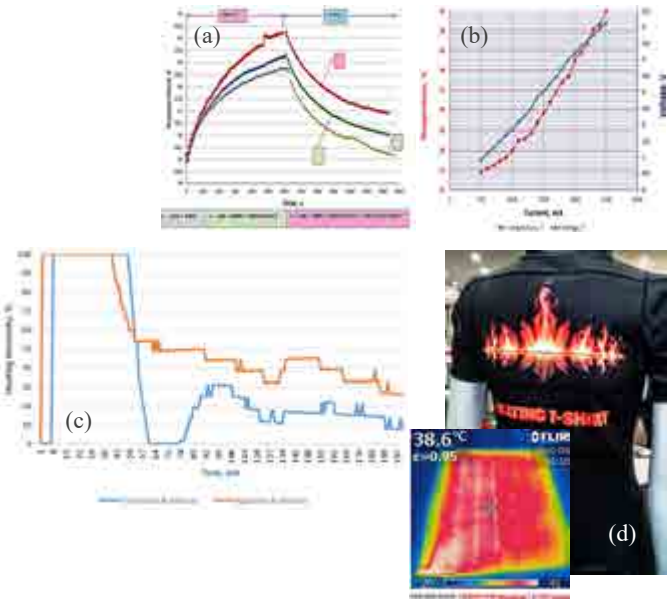


Fig. 2. (a) Heating behaviour of knitted fabric on human skin (internal thermocouple sensor, voltage 5V).
(b) Temperature and current dependences of isolated heating element on voltage.
(c) Heating intensity (%) of upper and lower heating elements in first 200 sec.
(d) Thermographic view of T-shirts with two heating elements.

Projects

Lithuanian-Swiss cooperation programme
R&D project "Aerosol in Lithuania: Investigation of primary–secondary and regional–local contributions to particulate matter in the south-eastern Baltic region" (AEROLIT)

V. Ulevičius

Lithuanian-Swiss cooperation programme
R&D project "Single-Cell-on-a-Chip Platform for Metabolite Sensing and Integrated Analysis"

R. Valiokas

7th Framework programme project
"Polymer-Carbon Nanotubes Active Systems for Photovoltaics"

L. Valkūnas

7th Framework programme project
"Hub of Application Laboratories for Equipment Assessment in Laser Based Manufacturing" (APPOLO)

G. Račiukaitis

7th Framework programme project
"Novel Type of Terahertz Devices"

A. Krotkus

Research Executive Agency (REA), delegated by the European Commission project "Camelina&crambe Oil Crops as Sources for Medium-chain Oils for Specialty Oleochemicals" (COSMOS)

S. Asadauskas

Research Executive Agency (REA), delegated by the European Commission project "Energy losses in nitride light-emitting diodes" (NITRIDE-SRH)

A. Alkauskas

European Commision European Atomic Energy Community (Euratom) project "Baltic Region Initiative for Long Lasting Innovative Nuclear Technologies" (BRILLIANT)

L. Juodis

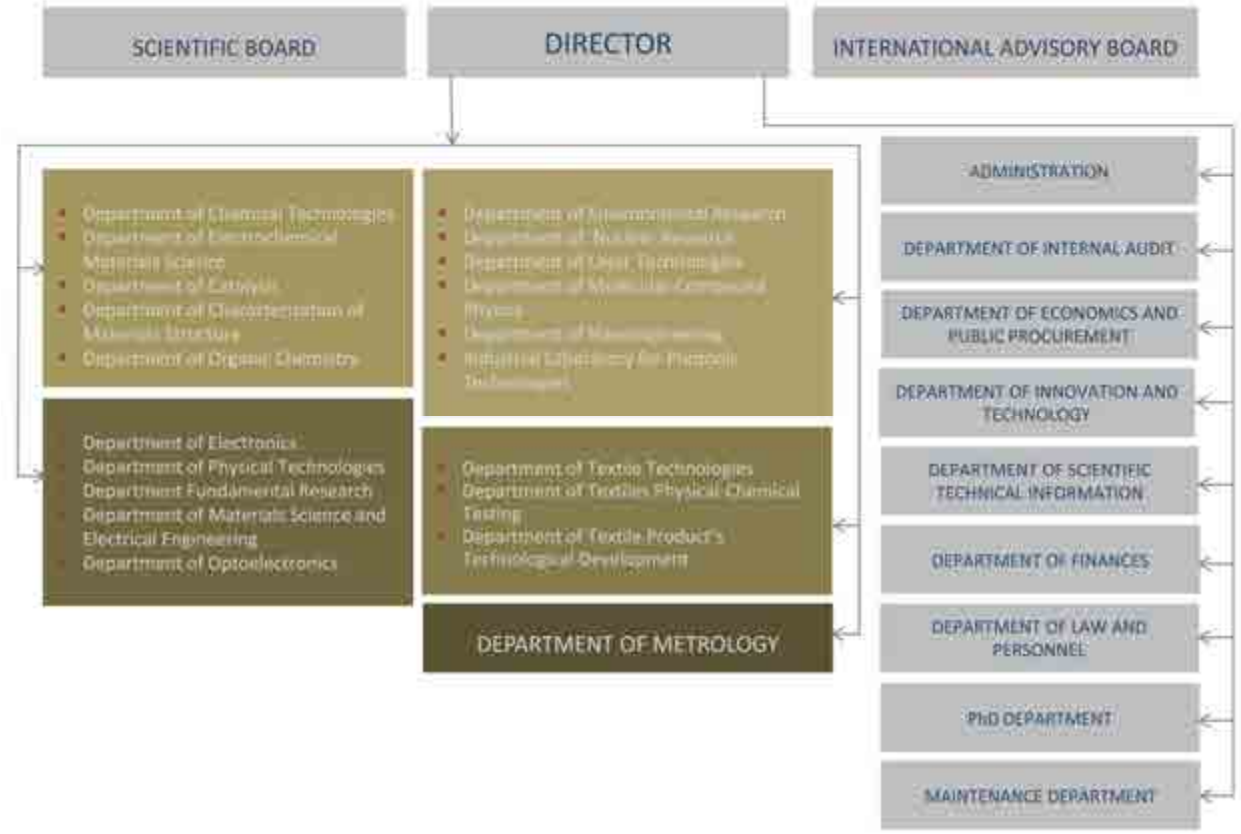
European Space Agency (ESA) project
"Bismides for Infrared photodetector" (BIRD)

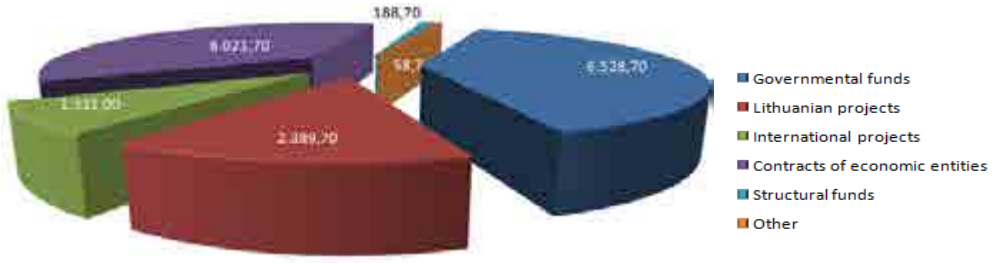
A. Krotkus

Horizon 2020 programme project
“PHotonics enhanced fAB LABS supporting the next revolution in digitalization“ (PHABLABS)

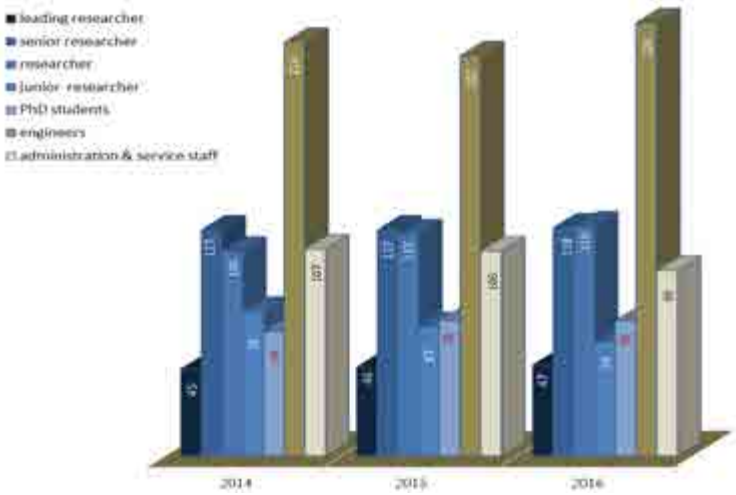
S. Orlovas

Structure and statistics





Budget of FTMC 2016, kEur



Staff dynamics

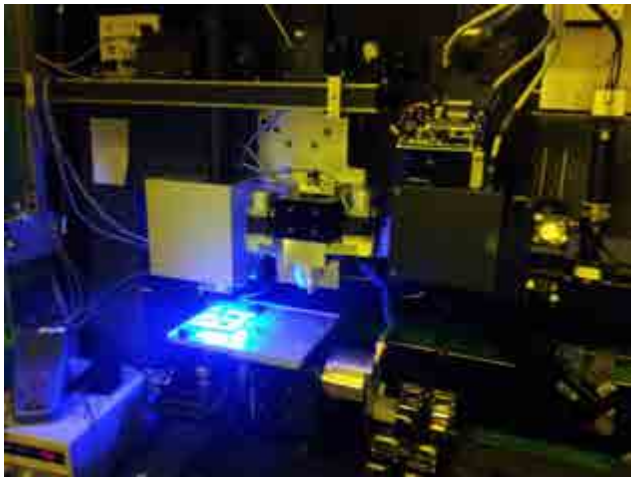
Open access centers

OAC for electron microscopy, X-ray diffractometry and spectrometry

has well developed infrastructure and experienced staff for the characterisation of solid materials using SEM, SEM-FIB, TEM, EDX, XRD, HRXRD, WDXRF, XPS techniques.

Available equipment:

- Scanning electron microscopes: Helios Nanolab 650, EVO-50;
- Transmission electron microscope Tecnai G2 F20 X-TWIN;
- X-ray diffractometers: SmartLab (Rigaku), D8 Advance (Bruker);
- X-ray fluorescence spectrometer (WDXRF) Axios mAX (Panalytical);
- X-ray photoelectron spectrometer ESCALAB-MKII;
- Carbon and sulphur analyser CS-2000.



OAC of processing technologies BALTFAB

is a joint open user facility between Laser technologies and Nano-engineering departments, offering a full range of nano/micro and macro fabrication as well as laser patterning, marking and cutting on any required material. State of the art Laser-fab is equipped with full variety of industrial ns, ps and fs lasers. The team is experts to set-up, test and develop laser micro-machining processes and systems. Soft nano-lithography tools for rapid creation of nano-structures are tested to be live cell compatible. The patterns are routinely applied to improve the bio-compatibility of medical devices. The team is developing tools for detection of molecules on surfaces, to fasten the testing and evaluation of cells or drugs. More: see www.baltfab.com

Services:

- **Laser processing**: in-Glass marking; laser beam interference ablation; laser direct writing; ultrashort pulse laser ablation.
- **Molecular**: dip pen nanolithography; microcontact printing; piezoelectric inkjet printing; colloidal nanolithography.
- **Analytical**: bio AFM; electrochemical sensors; imaging surface plasmon ellipsometry.

Available equipment:

- Ultra short pulse Laser stations for rent and user training services.
- Dip pen nanolithography and imaging ellipsometry for creating and imaging of molecular surfaces.

OAC for prototype formation and integration

Clean room technology for prototyping of semiconductor based devices

Based on collaboration between the Departments for Physical Technologies and Optoelectronics, a complete cycle of the clean room (CR) microfabrication line (see Fig. 1a) has started to function which is acceptable to produce the working models and the demonstration prototypes of chemical and photo-sensitive devices as single units and as limited batches of products. The prototyping of innovative devices is based on a few key enabling technologies including the PECVD/CVD for synthesis of 2D materials, namely graphene and MoS2, multimode magnetron sputtering for deposition of multicomponent functional films and molecule beam epitaxy for GaAs based optoelectronic devices.

The CR services include the following:

- CR (ISO7–ISO5 about 300 m^2) operations,
- photolithography,
- laser lithography,
- wet chemical processing,
- thermal processing,
- metal and oxide coatings,
- assemblage and testing.

Characterisation and testing of prototypes

The R&D projects in the APC PFI can range from proof of concepts (TRL – Technological Readiness Level- 3), validation of technologies in laboratory (TRL 4) or relevant environment (TRL 5), and up to demonstration in relevant environment (TRL 6). In specific cases the collaboration can reach prototyping in operational environment (TRL 7). For this we use the methods acceptable to characterize the components and devices at the nanometer scale level and at the level of complete unit.

The characterization includes:

- topography, force spectroscopy, tunneling current spectroscopy by scanning probe microscopy,
- standard I-V and C-V characteristics in the dc- and ac-modes by the probe station,
- photovoltaic parameters with the A1.5 solar source by special set-up,
- gas response in the synthetic atmosphere under strictly controlled conditions by gas flow control system.

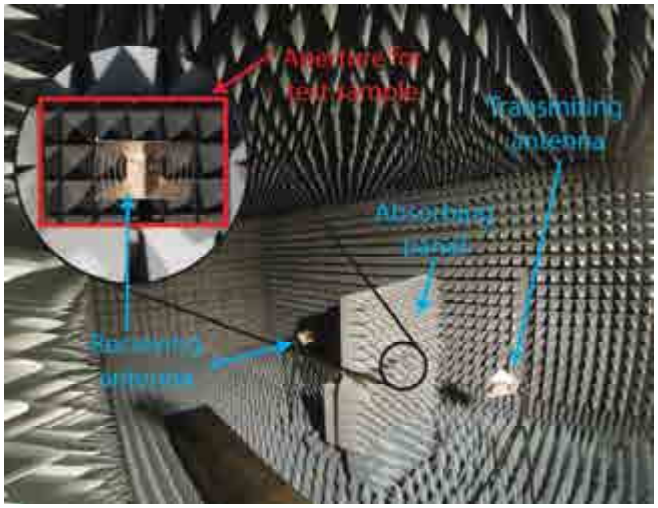
We also can carry out special set of tests for the response and resistivity to the microwave irradiation.

OAC for converse and chemical coatings

specializes in aluminum and its alloys anodation, galvanic precious metals plating and related fields. The services provided: electrodeposition of protective, decorative as well as technical converse (anodic) coatings, structural etching of decoration elements, adsorption coloring of anodized surfaces, modification of aluminum and its alloys surfaces with a passivation film that provides the required conductivity, protection and other properties, chemical deposition of passivation coatings onto alloy steels.

Available equipment:

- Experimental equipment for environment-friendly galvanic processes, anodizing line.
- Chemical passivation line for chromium-free passivation process of aluminium and its alloys, IRIDITE NCP.



Setup for microwave signal transmission, reflection and absorption in an anechoic chamber.

Microwave transmission, reflection and absorption

In a new microwave anechoic chamber of the Center for Physicals Sciences and Technology we developed a setup for microwave transmission and reflection measurement in a frequency range from 1 GHz to 18 GHz. Configuration of the measurement setup with transmitting and receiving antennas is shown in Fig. 2. Measured sample is placed in the aperture of the absorbing panel. Using this technique it is possible to measure microwave properties of various modern materials: windowpanes, absorbing textiles, shielding materials, etc.

Events

THE OPENING OF FTMC

/2016 03 15/

President of the Republic of Lithuania Dalia Grybauskaitė, the Prime Minister Algirdas Butkevičius, and Jose Angel Gurria, General Secretary of the Organisation for Economic Co-operation and Development (OECD), have started the opening ceremony with their welcoming speeches. Delegations of the European Commission, CERN, MPs, and Ministers of the Republic of Lithuania, Diplomatic Corps, City Mayors and many other honorable guests joined this exciting celebration.

ANNUAL FTMC CONFERENCE

/ 2016 02 10-11/

Reports on development of Long-Term Programs of scientific research and experimental development have been presented by the program leaders. Invited talks were given on the most interesting results obtained in 2015. G. Valušis, the Director of FTMC, presented his annual report mentioning the achievements of the year and nominating best scientists.

CONFERENCE “CHEMISTRY AND CHEMICAL TECHNOLOGY 2016”

/ 2016 04 28-29/

The year 2016 marks 210th anniversary of the publication of the first theory of electrolysis proposed by Theodor Grotthuss (1785 – 1822), a scientist who spent most of his life in Lithuania. The conference was aimed at bringing together scientists to discuss different topics in modern electrochemical, chemical and technological research. The topics of the conference included: experimental and theoretical aspects of charge transfer at electrochemical interfaces, electrochemical material science, nanoplating and nanostructured materials, bioelectrochemistry, chemistry

and technology of inorganic materials, chemistry of organic materials, analytical and environmental chemistry, polymer chemistry and technology. The conference brought together 260 scientists (mostly young researchers) from 14 countries.

PRESIDENT OF ROMANIA KLAUS IOHANNIS VISITED FTMC

/2016 05 18/

The guests were acquainted with the technological innovations of Lithuania by demonstrating some successful examples of research and business collaboration. As mentioned by G. Valušis, the Director of FTMC, in a geographically small place a huge additional value is created due to the synergy of science and business.

6TH FTMC CONFERENCE FOR DOCTORANTS AND YOUNG SCIENTISTS

/2016 10 26-27/

Young scientists and doctorants presented their research in physics, chemistry, material science and electro-engineering.

DAY OF PHOTONICS AT FTMC

/2016 10 21/

The event took place at the facilities of Institute of Physics, FTMC. The participants visited the laboratories of Laser technology Division of FTMC as well as companies belonging to the cluster of Laser and Engineering Technologies. They listened to the lectures on laser application, participated in discussions and evidenced the fascinating laser show. The lectures were given by prof. Y. Nishijima, prof. R. Gadonas, dr. M. Gedvilas and others.

Awards

Albertas Malinauskas – For scientific achievements

During a long time of his research activity, which included as periods of a heavy deficit of available equipment and materials, as well as decent facilities for experimental work during his research stays abroad, A. Malinauskas carried out many significant experiments. His research interests lie at the intersection of different branches of chemistry – physical, organic and electrochemistry – spiced with a little bit of physics (spectroscopy) and biochemistry (enzymes). The publications of A. Malinauskas have been internationally recognized and well cited.

Gediminas Niaura – For outstanding publications

The research of physical chemist G. Niaura is dedicated to vibrational spectroscopy of nanomaterials, biomolecules, self-assembled monolayers, and interfaces, focussing on electrochemical surface enhanced Raman spectroscopy. He studies the molecular processes at electrified interfaces in order to elucidate the architecture and function of adsorbed molecules and ions.

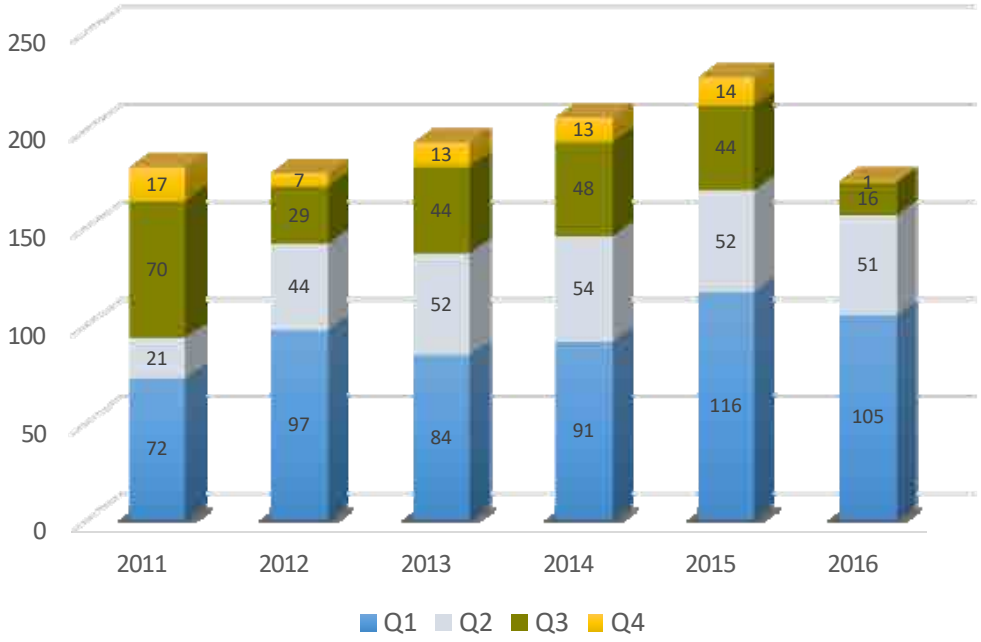
Algirdas Matulis – For lifetime achievements

A. Matulis graduated from Physics Department of Moscow University as an experimentalist, but the courses of quantum mechanics in Adolfas Jucis laboratory of atomic spectroscopy and work in Semiconductor Physics Institute, Vilnius made him a wide scope theorist in condensed matter and semiconductor physics. He studied electron scattering by optical phonons, the effect resulting in the anisotropy of the distribution function and non-trivial transport properties. He was also interested in quantum properties of the electron system when the electron-phonon interaction causes the occurrence of bounded electron-optical phonon states. His studies of low dimensional electron systems, non-relativistic and Dirac electron dynamics and spectra in non-homogeneous magnetic fields, the works on quantum dots and graphene contributed significantly to quantum nano-physics. Several generations of Lithuanian physicists have been learning from Matulis' text-books on different fields of physics. His seminars and lectures are examples of how the most complicated problems could be presented in a simple and attractive way.

Arūnas Šetkus – For innovations

Key enabling technologies together with an infrastructure devoted to the manufacturing of conventional semiconductor devices opened fascinating possibilities for development of innovative devices detecting external influences and compatible with the modern systems dedicated to the direct communication between devices or so called the Internet of things. A. Šetkus was responsible for the setting of technological equipment at working conditions in the new Center for Physical Sciences and Technology. He gathered together the ambitious team of young scientists for development of original technologies. The team demonstrated the ability to manufacture hybrid structures that include functional coatings, two-dimensional materials and biological objects, the ability which stimulates a novel synergy between the physical science, technology and biotechnology. Special focus on the applied activities opens new gates not only for joint actions with the commercial companies but also creates a basis for establishment of novel start-up companies.

Publications



Publications with FTMC affilations in 2016 in top quartile (Q1) journals

1. Balčiauskas, L.; Skipitytė, R.; Jasiulionis, M.; Trakimas, G.; Balčiauskienė, L.; Remeikis, V. The impact of Great Cormorants on biogenic pollution of land ecosystems : stable isotope signatures in small mammals // Science of the total environment. ISSN 0048-9697. Vol. 565 (2016), p. 376-383.
2. Abdi-Jalebi, M.; Dar, M. I.; Sadhanala, A.; Senanayak, S.P.; Franckevičius, M.; Arora, N.; Hu, Y.; Nazeeruddin, M. K.; Zakeeruddin, S. M.; Grätzel, M.; Friend, R. H. Impact of monovalent cation halide additives on the structural and optoelectronic properties of $CH_3NH_3PbI_3$ perovskite // Advanced energy materials. ISSN 1614-6832. Vol. 6, iss. 10 (2016), p. art. no. 1502472 [1-10].
3. Devižis, A.; De Jonghe-Risse, J.; Hany, R.; Nüesch, F.; Jenatsch, S.; Gulbinas, V.; Moser, J.-E. Dissociation of charge transfer states and carrier separation in bilayer organic solar cells: A time-resolved electroabsorption spectroscopy study // Journal of the American Chemical Society. ISSN 0002-7863. Vol. 137, iss. 25 (2015), p. 8192–8198.
4. Meloni, S.; Moehl, T.; Tress, W.; Franckevičius, M.; Saliba, M.; Lee, Y. H.; Gao, P.; Nazeeruddin, M. K.; Zakeeruddin, S. M.; Rothlisberger, U.; Graetzel, M. Ionic polarization-induced current-voltage hysteresis in $CH_3NH_3PbX_3$ perovskite solar cells // Nature communications. ISSN 2041-1723. Vol. 7 (2016), p. Art. no. 10334 [1-9].
5. Shumakova, V.; Malevich, P.; Ališauskas, S.; Voronin, A.; Zheltikov, A.M.; Faccio, D.; Kartashov, D.; Baltuška, A.; Pugžlys, A. Multi-millijoule few-cycle mid-infrared pulses through nonlinear self-compression in bulk // Nature communications. ISSN 2041-1723. Vol. 7, (2016), p. art. no. 12877 [1-6].
6. Doherty, M.W.; Meriles, C.A.; Alkauskas, A.; Fedder, H.; Sellars, M.J.; Manson, N.B. Towards a room-temperature spin quantum bus in diamond via electron photoionization, transport, and capture // Physical review X. ISSN 2160-3308. Vol. 6, iss.4 (2016), p. art. no. 041035 [1-14].
7. Wang, H.; Valkūnas, L.; Cao, T.; Whittaker-Brooks, L.; Fleming, G. R. Coulomb screening and coherent phonon in methylammonium lead iodide perovskites // Journal of physical chemistry letters. ISSN 1948-7185. Vol. 7, no. 16 (2016), p. 3284-3289.
8. Butkus, V.; Dong, H.; Fleming, G. R.; Abramavičius, D.; Valkūnas, L. Disorder-induced quantum beats in two-dimensional spectra of excitonically coupled molecules // Journal of physical chemistry letters. ISSN 1948-7185. Vol. 7, no. 2 (2016), p. 277–282.
9. Farooq, S.; Chmeliov, J.; Trinkūnas, G.; Valkūnas, L.; Van Amerongen, H. Is there excitation energy transfer between different layers of stacked photosystem-II-containing thylakoid membranes? // Journal of physical chemistry letters. ISSN 1948-7185. Vol. 7, no. 7 (2016), p. 1406-1410.
10. Sofen, E.D.; Bowdalo, D.; Evans, M.J.; Apadula, F.; Bonasoni, P.; Cupeiro, M.; Ellul, R.; Galbally, I. E.; Girgždienė, R.; Luppo, S.; Mimouni, M.; Nahas, A. C.;

Saliba, M.; Tørseth, K.. Gridded global surface ozone metrics for atmospheric chemistry model evaluation // Earth system science data. ISSN 1866-3508. Vol. 8 (2016), p. 41-59.

11. Chmeliov, J.; Narkeliūnas, J.; Graham, M. W.; Fleming, G. R.; Valkūnas, L. Exciton-exciton annihilation and relaxation pathways in semiconducting carbon nanotubes // Nanoscale. ISSN 2040-3364. Vol. 8, iss. 3 (2016), p. 1618-1626.

12. Leyman, R.R.; Gorodetsky, A.; Bazieva, N.; Molis, G.; Krotkus, A.; Clarke, E.; Rafailov, E.U. Quantum dot materials for terahertz generation applications // Laser & photonics reviews. ISSN 1863-8880. Vol. 10, iss.5 (2016), p. 772-779.

13. Dinda, S.; Suresh, V.; Thoniyot, P.; Balčytis, A.; Juodkazis, S.; Krishnamoorthy, S. Engineering 3D nanoplasmonic assemblies for high performance spectroscopic sensing // ACS applied materials & interfaces. ISSN 1944-8244. Vol. 7, iss. 50 (2015), p. 27661–27666.

14. Bi, Do.; Mishra, A.; Gao, P.; Franckevičius, M.; Steck, Ch.; Zakeeruddin, Sh. M.; Nazeeruddin, M.K.; Bäuerle, P.; Grätzel, M.; Hagfeldt, A. High-efficiency perovskite solar cells employing a S,N-heteropentacene-based D-A hole-transport material // ChemSusChem. ISSN 1864-5631. Vol. 9, iss. 5 (2016), p. 433-438.

15. Lazauskas, A.; Baltrušaitis, J.; Puodžiukynas, L.; Andrulevičius, M.; Bagdžiūnas, G.; Volyniuk, D.; Meškinis, Š.; Niaura, Ge.; Tamulevičius, T.; Jankauskaitė, V. Characterization of urea derived polymeric carbon nitride and resultant thermally vacuum deposited amorphous thin films: Structural, chemical and photophysical properties // Carbon. ISSN 0008-6223. Vol. 107 (2016), p. 415-425.

16. Kanosue, K.; Augulis, R.; Peckus, D.; Karpič, R.; Tamulevičius, T.; Tamulevičius, S.; Gulbinas, V.; Ando, S. Polyimide and imide compound exhibiting bright red fluorescence with very large stokes shifts via excited-state intramolecular proton transfer II. Ultrafast proton transfer dynamics in the excited state // Macromolecules. ISSN 0024-9297. Vol. 49, iss. 5 (2016), p. 1848-1857.

17. Shotan, Z.; Jayakumar, H.; Considine, C.R.; Mackoit, M.; Fedder, H.; Wrachtrup, J.; Alkauskas, A.; Doherty, M.W.; Menon, V.M.; Meriles, C.A. Photoinduced modification of single-photon emitters in hexagonal boron nitride // ACS Photonics. ISSN 2330-4022. Vol. 3, iss.12 (2016), p. 2490-2496.

18. Čeburnis, D.; Mašalaitė-Nalivaikė, A.; Ovadnevaite, J.; Garbaras, A.; Remeikis, V.; Maenhaut, W.; Claeys, M.; Sciare, J.; Baisnée, D.; O'Dowd, C.D. Stable isotopes measurements reveal dual carbon pools contributing to organic matter enrichment in marine aerosol // Scientific reports. ISSN 2045-2322. Vol. 6 (2016), p. art. no. 36675 [1-6].

19. Gedvilas, M.; Ratautas, K.; Kacar, E.; Stankevičienė, I.; Jagminienė, A.; Norkus, E.; Li Pira, N.; Račiukaitis, G. Colour-difference measurement method for evaluation of quality of electrolessly deposited copper on polymer after laser-induced selective activation // Scientific reports. ISSN 2045-2322. Vol. 6 (2016), p. art. no. 22963 [1-8].

20. Hashimoto, Y.; Seniutinas, G.; Balčytis, A.; Juodkazis, S.; Nishijima, Y. Au-Ag-Cu nano-alloys: tailoring of permittivity // Scientific reports. ISSN 2045-2322. Vol. 6 (2016), p. art. no. 25010 [1-9].

21. Janulevičius, M.; Marmokas, P.; Misevičius, M.; Grigorjevaitė, J.; Mikoliūnaitė, L.; Šakirzanovas, S.; Katelnikovas, A. Luminescence and luminescence quenching of highly efficient Y2Mo4O15:Eu3+ phosphors and ceramics // Scientific reports. ISSN 2045-2322. Vol. 6 (2016), p. art. no. 26098 [1-12].

22. Romanov, S.G.; Orlovas, Se.; Ploss, D.; Weiss, C.K.; Vogel, N.; Peschel, U. Engineered disorder and light propagation in a planar photonic glass // Scientific reports. ISSN 2045-2322. Vol. 6 (2016), p. art. no. 27264 [1-10].

23. Abramavičius, V.; Pranculis, V.; Melianas, A.; Inganäs, O.; Gulbinas, V.; Abramavičius, D. Role of coherence and delocalization in photo-induced electron transfer at organic interfaces // Scientific reports. ISSN 2045-2322. Vol. 6 (2016), p. art. no. 32914 [1-7].

24. Jagminas, A.; Niaura, G.; Žalnėravičius, R.; Trusovas, R.; Račiukaitis, G.; Jasulaitienė, V. Laser light induced transformtion of molybdenum disulphide-based nanoplatelet arrays // Scientific reports. ISSN 2045-2322. Vol. 6 (2016), p. art. no. 37514 [1-9].

25. Fülöp, J.A.; Polónyi, Gy.; Monoszlai, B.; Andriukaitis, G.; Balciunas, T.; Pugžlys, A.; Arthur, G.; Baltuška, A.; Hebling, J.. Highly efficient scalable monolithic semiconductor terahertz pulse source // Optica. ISSN 2334-2536. Vol. 3, iss.10 (2016), p. 1075-1078.

26. Mitrofanov, AV.; Voronin, A.A.; Sidorov-Biryukov, D.A.; Mitryukovskiy, S.I.; Fedotov, A.B.; Serebryannikov, E.E.; Meshchankin, D. V.; Shumakova, V.; Ališauskas, S.; Pugžlys, A.; Panchenko, V.Ya.; Baltuška, A.; Zheltikov, A.M. Subterawatt few-cycle mid-infrared pulses from a single filament // Optica. ISSN 2334-2536. Vol. 3, iss.3 (2016), p. 299-302.

27. Trusovas, R.; Račiukaitis, G.; Niaura, G.; Barkauskas, J.; Valušis, G.; Pauliukaitė, R. Recent advances in laser utilization in the chemical modification of graphene oxide and its applications // Advanced optical materials. ISSN 2195-1071. Vol. 4, iss. 1 (2016), p. 37-65.

28. Ulevičius, V.; Byčenkienė, S.; Bozzetti, C.; Vlachou, A.; Plauškaitė-Šukienė, K.; Mordas, G.; Dudoitis, V.; Abbaszade, G.; Remeikis, V.; Garbaras, A.; Mašalaitė, A.; Blees, J.; Fröhlich, R.; Dällenbach, K.R.; Canonaco, F.; Slowik, J.G.; Dommen, J.; Zimmermann, R.; Schnelle-Kreis, J.; Salazar, G.A.; Agrios, K.; Szidat, S.; El Haddad, I.; Prévôt, A.S.H. Fossil and non-fossil source contributions to atmospheric carbonaceous aerosols during extreme spring grassland fires in Eastern Europe // Atmospheric chemistry and physics. ISSN 1680-7316. Vol. 16, iss. 9 (2016), p. 5513-5529.

29. Zubovas, K.; Bourne, M.A.; Nayakshin, S. A simple way to improve AGN feedback prescription in SPH simulations // Monthly notices of the Royal astronomical society. ISSN 0035-8711. Vol. 457, iss.1 (2016), p. 496-509.

30. Zubovas, K.; King, A. The small observed scale of AGN-driven outflows, and inside-out disc quenching // Monthly notices of the Royal astronomical society. ISSN 0035-8711. Vol. 462, iss.4 (2016), p. 4055-4066.

31. German, N.; Kaušaitė-Minkštimienė, A.; Ramanavičius, A.; Semashko, T.; Mikhailova, R.; Ramanavičienė, A. The use of different glucose oxidases for the development of an amperometric reagentless glucose biosensor based on gold nanoparticles covered by polypyrrole // Electrochimica acta. ISSN 0013-4686. Vol. 169 (2015), p. 326-333.

32. Kežionis, A.; Petrulionis, D.; Kazakevičius, E.; Kazlauskas, S.; Žalga, A.; Juškėnas, R. Charge carrier relaxation phenomena and phase transition in La2Mo2O9 ceramics investigated by broadband impedance spectroscopy // Electrochimica acta. ISSN 0013-4686. Vol. 213 (2016), p. 306-313.

33. Radzevič, A.; Niaura, G.; Ignatjev, I.; Rakickas, T.; Celiešiūtė, R.; Pauliukaitė, R. Electropolymerisation of the natural monomer riboflavin and its characterisation // Electrochimica acta. ISSN 0013-4686. Vol. 222 (2016), p. 1818-1830.

34. Ivanauskas, F.; Morkvėnaitė-Vilkončienė, I.; Astrauskas, R.; Ramanavičius, A. Modelling of scanning electrochemical microscopy at redox competition mode using diffusion and reaction equations // Electrochimica acta. ISSN 0013-4686. Vol. 222 (2016), p. 347-354.

35. Morkvėnaitė-Vilkončienė, I.; Ramanavičienė, A.; Ramanavičius, A. 9,10-Phenanthrenequinone as a redox mediator for the imaging of yeast cells by scanning electrochemical microscopy // Sensors and actuators. B, Chemical. ISSN 0925-4005. Vol. 228 (2016), p. 200-206.

36. Talaikis, M.; Eicher-Lorka, O.; Valinčius, G.; Niaura, G. Water-induced structural changes in the membrane-anchoring monolayers revealed by isotope-edited SERS // Journal of physical chemistry. C. ISSN 1932-7447. Vol. 120 (2016), p. 22489-22499.

37. Jagminas, A.; Kačiulis, S.; Klimas, V.; Rėza, A.; Mickevičius, S.; Soltani, P. Fabrication of graphene–alumina heterostructured films with nanotube morphology // Journal of physical chemistry. C. ISSN 1932-7447. Vol. 120, iss. 17 (2016), p. 9490-9497.

38. Pranculis, V.; Ruseckas, A.; Vithanage, A.D.; Hedley, J.G.; Samuel, I.D.W.; Gulbinas, V. Influence of blend ratio and processing additive on free carrier yield and mobility in PTB7:PC71BM photovoltaic solar cells // Journal of physical chemistry. C. ISSN 1932-7447. Vol. 120, iss. 18 (2016), p. 9588–9594.

39. Bertašius, V.; Mastria, R.; Rizzo, A.; Gigli, G.; Giansante, C.; Gulbinas, V. Charge carrier generation and extraction in hybrid polymer/quantum dot solar cells // Journal of physical chemistry. C. ISSN 1932-7447. Vol. 120, iss. 26 (2016), p. 14356–14364.

40. Baitimirova, M.; Viter, R.; Andzane, J.; van der Lee, A.; Voiry, D.; Iatsunskyi, I.; Coy, E.; Mikoliūnaitė, L.; Tumėnas, S.; Załęski, K.; Balevičius, Z.; Balevičiūtė, I.; Ramanavičienė, A.; Ramanavičius, A.; Jurga, S.; Erts, D.; Bechelany, M. Tuning of structural and optical properties of graphene/ZnO nanolaminates // Journal of physical chemistry. C. ISSN 1932-7447. Vol. 120, iss. 41 (2016), p. 23716-23725.

41. Viter, R.; Iatsunskyi, I.; Fedorenko, V.; Tumėnas, S.; Balevičius, Z.; Ramanavičius, A.; Balme, S.; Kempiński, M.; Nowaczyk, G.; Jurga, S.; Bechelany, M. Enhancement of electronic and optical properties of ZnO/Al2O3 nanolaminate coated electrospun nanofibers // Journal of physical chemistry. C. ISSN 1932-7447. Vol. 120, iss. 9 (2016), p. 5124-5132.

42. Ibenskas, A.; Šimėnas, M.; Tornau, E. Numerical engineering of molecular self-assemblies in a binary system of trimesic and benzenetribenzoic acids // Journal of physical chemistry. C. ISSN 1932-7447. Vol. 120, iss.12 (2016), p. 6669–6680.

43. Paraecattil, A.A.; De Jonghe-Risse, J.; Pranculis, V.; Teuscher, J.; Moser, J.-E. Dynamics of photocarrier separation in MAPbI3 perovskite multigrain films under a quasistatic electric field // Journal of physical chemistry. C. ISSN 1932-7447. Vol. 120, iss.35 (2016), p. 19595-19602.

44. Šimėnas, M.; Balčiūnas, S.; Maczka, M.; Banys, J.; Tornau, E. Structural phase transition in perovskite metal–formate frameworks: a Potts-type model with dipolar interactions // Physical chemistry chemical physics. ISSN 1463-9076. Vol. 18, iss. 27 (2016), p. 18528-18535.

45. Gruber, M.J.; Xu, P.; Chmeliov, J.; Krüger, T. P. J.; Alexandre, M.T.A.; Valkūnas, L.; Croce, R.; van Grondelle, R. Dynamic quenching in single photosystem II supercomplexes // Physical chemistry chemical physics. ISSN 1463-9076. Vol. 18, iss. 37 (2016), p. 25852-25860.

46. Abramavičius, D.; Valkūnas, L. Role of coherent vibrations in energy transfer and conversion in photosynthetic pigment–protein complexes // Photosynthesis research. ISSN 0166-8595. Vol. 127, iss. 1 (2016), p. 33-47.

47. Chmeliov, J.; Trinkūnas, G.; Van Amerongen, H.; Valkūnas, L. Excitation migration in fluctuating light-harvesting antenna systems // Photosynthesis research. ISSN 0166-8595. Vol. 127, iss. 1 (2016), p. 49-60.

48. Streckaitė, S.; Karpič, R.; Gruodis, A.; Dehaen, W.; Van Snick, S.; Kirkus, M.; Grigalevičius, S.; Gražulevičius, J.V.; Gulbinas, V. Fluorescence quenching of indolo[3,2-b]carbazole compounds by conformational motions of attached substituents // Dyes and pigments. ISSN 0143-7208. Vol. 133 (2016), p. 120-126.

49. Alkauskas, A.; Dreyer, C.E.; Lyons, J.L.; Van de Walle, C.G. Role of excited states in Shockley-Read-Hall recombination in wide-band-gap semiconductors // Physical review. B. ISSN 1098-0121. Vol. 93, iss. 20 (2016), p. art. no. 201304 [1-5].

50. Gečys, P.; Markauskas, E.; Žemaitis, A.; Račiukaitis, G. Variation of P2 series interconnects electrical conductivity

in the CIGS solar cells by picosecond laser-induced modification // Solar energy. ISSN 0038-092X. Vol. 132 (2016), p. 493-502.

51. Stirkė, A.; Apetrei, R.-M.; Kirsnytė, M.; Dedelaitė, L.; Bondarenka, V.; Jasulaitienė, V.; Pučetaitė, M.; Selskis, A.; Carac, G.; Bahrim, G.; Ramanavičius, A. Synthesis of polypyrrole microspheres by Streptomyces sp. // Polymer. ISSN 0032-3861. Vol. 84 (2016), p. 99-106.

52. Juodis, L.; Filistovič, V.; Maceika, E.; Remeikis, V. Analytical dispersion model for the chain of primary and secondary air pollutants released from point source // Atmospheric environment. ISSN 1352-2310. Vol. 128 (2016), p. 216-226.

53. Raudonytė-Svirbutavičienė, E.; Mikoliūnaitė, L.; Drabavičius, A.; Juškėnas, R.; Šakirzanovas, S.; Jüstel, T.; Katelnikovas, A. Photochemical synthesis of CeO2 nanoscale particles using sodium azide as a photoactive material: effects of the annealing temperature and polyvinylpyrrolidone addition // RSC advances. ISSN 2046-2069. Vol. 6, iss. 108 (2016), p. 107065-107074.

54. Juodkazytė, J.; Seniutinas, G.; Šebeka, B.; Savickaja, I.; Malinauskas, T.; Badokas, K.; Juodkazis, K.J.; Juodkazis, S. Solar water splitting: Efficiency discussion // International journal of hydrogen energy. ISSN 0360-3199. Vol. 41, iss. 28 (2016), p. 11941–11948.

55. Jagminas, A.; Naujokaitis, A.; Žalnėravičius, R.; Jasulaitienė, V.; Valušis, G. Tuning the activity of nanoplatelet MoS2-based catalyst for efficient hydrogen evolution via electrochemical decoration with Pt nanoparticles // Applied surface science. ISSN 0169-4332. Vol. 385 (2016), p. 56-62.

56. Masim, F.C.P.; Liu, H.-Li; Porta, M.; Yonezawa, T.; Balčytis, A.; Juodkazis, S.; Hsu, W.-H.; Hatanaka, K. Enhanced photoacoustics from gold nano-colloidal suspensions under femtosecond laser excitation // Optics express. ISSN 1094-4087. Vol. 24, iss. 13 (2016), p. 14781-14792.

57. Balčytis, A.; Hakobyan, D.; Gabalis, M.; Žukauskas, A.; Urbonas, D.; Malinauskas, M.; Petruškevičius, R.; Brasselet, E.; Juodkazis, S. Hybrid curved nano-structured micro-optical elements // Optics express. ISSN 1094-4087. Vol. 24, iss. 15 (2016), p. 16988-16998.

58. Masim, F.C.P.; Hsu, W.-H.; Tsai, C.-H.; Liu, H.-Li; Porta, M.; Nguyen, M. T.; Yonezawa, T.; Balčytis, A.; Wang, X.; Juodkazis, S.; Hatanaka, K. MHz-ultrasound generation by chirped femtosecond laser pulses from gold nano-colloidal suspensions // Optics express. ISSN 1094-4087. Vol. 24, iss. 15 (2016), p. 17050-17059.

59. Danilevičius, R.; Zaukevičius, A.; Budriūnas, R.; Michailovas, A.; Rusteika, N. Femtosecond wavelength-tunable OPCPA system based on picosecond fiber laser seed and picosecond DPSS laser pump // Optics express. ISSN 1094-4087. Vol. 24, iss. 15 (2016), p. 17532-17540.

60. Hsu, W.-H.; Masim, F. C.P.; Porta, M.; Nguyen, M.T.; Yonezawa, T.; Balčytis, A.; Wang, X.; Rosa, L.; Juodkazis, S.; Hatanaka, K. Femtosecond laser-induced hard X-ray generation in air from a solution flow of Au nano-sphere suspension using an automatic positioning system // Optics express. ISSN 1094-4087. Vol. 24, iss. 18 (2016), p. 19994-20001.

61. Michailovas, K.; Baltuška, A.; Pugžlys, A.; Smilgevičius, V.; Michailovas, A.; Zaukevičius, A.; Danilevičius, R.; Frankinas, S.; Rusteika, N. Combined Yb/Nd driver for optical parametric chirped pulse amplifiers // Optics express. ISSN 1094-4087. Vol. 24, iss. 19 (2016), p. 22261-22271.

62. Dudutis, J.; Gečys, P.; Račiukaitis, G. Non-ideal axicon-generated Bessel beam application for intra-volume glass modification // Optics express. ISSN 1094-4087. Vol. 24, iss. 25 (2016), p. 28433-28443.

63. Kaksis, E.; Almási, G.; Fülöp, J.A.; Pugžlys, A.; Baltuška, A.; Andriukaitis, G. 110-mJ 225-fs cryogenically cooled Yb:CaF2 multipass amplifier // Optics express. ISSN 1094-4087. Vol. 24, iss. 25 (2016), p. 28915-28922.

64. Huber, C.; Orlovas, S.; Banzer, P.; Leuchs, G. Influence of the substrate material on the knife-edge based profiling of tightly focused light beams // Optics express. ISSN 1094-4087. Vol. 24, iss. 8 (2016), p. 8214-8227.

65. Batrakov, K.; Kuzhir, P.; Maksimenko, S; Volynets, N.; Voronovich, S.; Paddubskaya, A.G.; Valušis, G.; Kaplas, T.; Svirko, Yu.; Lambin, Ph. Enhanced microwave-to-terahertz absorption in graphene // Applied physics letters. ISSN 0003-6951. Vol. 108, iss. 12 (2016), p. Art. no. 123101 [1-4].

66. Dreyer, C.E.; Alkauskas, A.; Lyons, J.L.; Speck, J.S.; Van de Walle, C.G. Gallium vacancy complexes as a cause of Shockley-Read-Hall recombination in III-nitride light emitters // Applied physics letters. ISSN 0003-6951. Vol. 108, iss. 14 (2016), p. art. no. 141101 [1-5].

67. Wickramaratne, D.; Shen, J.-X.; Dreyer, C.E.; Engel, M.; Marsman, M.; Kresse, G.; Marcinkevičius, S.; Alkauskas, A.; Van de Walle, C.G. Iron as a source of efficient Shockley-Read-Hall recombination in GaN // Applied physics letters. ISSN 0003-6951. Vol. 109, iss.16 (2016), p. art. no. 162107 [1-4].

68. Urbonas, D.; Balčytis, A.; Vaškevičius, K.; Gabalis, M.; Petruškevičius, R. Air and dielectric bands photonic crystal microringresonator for refractive index sensing // Optics letters. ISSN 0146-9592. Vol. 41, iss. 15 (2016), p. 3655-3658.

69. Malevich, P.; Kanai, T.; Hoogland, H.; Holzwarth, R.; Baltuška, A.; Pugžlys, A. Broadband mid-infrared pulses from potassium titanyl arsenate/zinc germanium phosphate optical parametric amplifier pumped by Tm, Ho-fiber-seeded Ho:YAG chirped-pulse amplifier // Optics letters. ISSN 0146-9592. Vol. 41, iss. 5 (2016), p. 930-933.

70. Jašinskas, V.; Gedvilas, M.; Račiukaitis, G.; Gulbinas, V. Background-free electric field-induced second harmonic generation with interdigitated combs of electrodes // Optics letters. ISSN 0146-9592. Vol. 41, iss.12 (2016), p. 2759-2762.

71. Kovalevich, T.; Ndao, A.; Suarez, M.; Tumėnas, S.; Balevičius, Z.; Ramanavičius, A.; Balevičiūtė, I.; Häyrinen, M.; Roussey, M.; Kuittinen, M.; Grosjean, T.; Bernal, M.-P. Tunable Bloch surface waves in anisotropic photonic crystals based on lithium niobate thin films // Optics letters. ISSN 0146-9592. Vol. 41, iss. 23 (2016), p. 5616-5619.

72. Juškėnas, R.; Niaura, G.; Mockus, Z.; Kanapeckaitė, S.; Giraitis, R.; Kondrotas, R.; Naujokaitis, A.; Stalnionis, G.; Pakštas, V.; Karpavičienė, V.M. XRD studies of an electrochemically co-deposited Cu-Zn-Sn precursor and formation of a Cu2ZnSnSe4 absorber for thin-film solar cells // Journal of alloys and compounds. ISSN 0925-8388. Vol. 655 (2016), p. 281-289.

73. Leinartas, K.; Juzeliūnas, E.; Staišiūnas, L.; Grigucevičienė, A.; Miečinskas, P.; Vaičiūnienė, J.; Jasulaitienė, V.; Kondrotas, R.; Juškėnas, R. Mg-Nb alloy films: Structure and stability in a balanced salt solution // Journal of alloys and compounds. ISSN 0925-8388. Vol. 661 (2016), p. 322-330.

74. Kosyak, V.; Znamenshchykov, Y.; Čerškus, A.; Gnatenko, Yu.P.; Grase, L.; Vecstaudza, J.; Medvids, A.; Opanasyuk, A.; Mezinskis, G.. Composition dependence of structural and optical properties of Cd1−xZnxTe thick films obtained by the close-spaced sublimation // Journal of alloys and compounds. ISSN 0925-8388. Vol. 682 (2016), p. 543-551.

75. Vernickaite, E.; Bubnienė, U.; Cesiulis, H.; Ramanavičius, A.; Podlahac, E.J. A hybrid approach to fabricated nanowire-nanoparticle composites of a Co-W alloy and Au nanoparticles // Journal of the Electrochemical Society. ISSN 0013-4651. Vol. 163, iss. 7 (2016), p. D344-D348.

76. Santos, D.M.F.; Balčiūnaitė, A.; Tamašauskaitė-Tamašiūnaitė, L.; Zabielaitė, A.; Jagminienė, A.; Stankevičienė, I.; Naujokaitis, A.; Norkus, E. AuCo/TiO2-NTs anode catalysts for direct borohydride fuel cells // Journal of the Electrochemical Society. ISSN 0013-4651. Vol. 163, iss.14 (2016), p. F1553-F1557.

77. Ratas, I.; Pyragas, K. Eliminating synchronization in bistable networks // Nonlinear dynamics. ISSN 0924-090X. Vol. 83, iss. 3 (2016), p. 1137-1151.

78. Kielė, E.; Senvaitienė, J.; Grigucevičienė, A.; Ramanauskas, R.; Raudonis, R.; Kareiva, A. Application of sol–gel method for the conservation of copper alloys // Microchemical journal. ISSN 0026-265X. Vol. 124 (2016), p. 623-628.

79. Dmukauskas, M.; Kadys, A.; Malinauskas, T.; Grinys, T.; Reklaitis, I.; Badokas, K.; Skapas, M.; Tomašiūnas, R.; Dobrovolskas, D.; Stanionytė, S.; Pietzonka, I.; Strassburg, M.; Lugauer, H. Influence of metalorganic precursors flow interruption timing on green InGaN multiple quantum wells // Journal of physics. D, Applied physics. ISSN 0022-3727. Vol. 49, iss.50 (2016), p. art. no. 505101 [1-7].

80. Žarkov, A.; Stanulis, A.; Šalkus, T.; Kežionis, A.; Jasulaitienė, V.; Ramanauskas, R.; Tautkus, S.; Kareiva, A. Synthesis of nanocrystalline gadolinium doped ceria via sol-gel combustion and sol-gel synthesis routes // Ceramics international. ISSN 0272-8842. Vol. 42, iss. 3 (2016), p. 3972–3988.

81. Kosyak, V.; Znamenshchykov, Y.; Čerškus, A.; Grase, L.; Gnatenko, Yu.P.; Medvids, A.; Opanasyuk, A.; Mezinskis, G.. Photoluminescence of CdZnTe thick films obtained by close-spaced vacuum sublimation // Journal of luminescence. ISSN 0022-2313. Vol. 171 (2016), p. 176-182.

82. Stanulis, A.; Katelnikovas, A.; van Bael, M.; Hardy, A.; Kareiva, A.; Justel, T. Photoluminescence of Pr3+-doped calcium and strontium stannates // Journal of luminescence. ISSN 0022-2313. Vol. 172 (2016), p. 323-330.

83. Auffray, E.; Augulis, R.; Borisevich, A.; Gulbinas, V.; Fedorov, A.; Korjik, M.; Lucchini, M.T.; Mechinsky, V.; Nargelas, S.; Songaila, E.; Tamulaitis, G.; Vaitkevičius, A.; Zazubovich, S.. Luminescence rise time in self-activated PbWO4 and Ce-doped Gd3Al2Ga3O12 scintillation crystals // Journal of luminescence. ISSN 0022-2313. Vol. 178 (2016), p. 54-60.

84. Kičas, S.; Gimževskis, U.; Melnikas, S. Post deposition annealing of IBS mixture coatings for compensation of film induced stress // Optical materials express. ISSN 2159-3930. Vol. 6, iss. 7 (2016), p. 2236-2243.

85. Rodaitė-Riševičienė, R.; Grincevičiūtė, N.; Selskis, A.; Snitka, V. Synthesis of hybrid graphene-porphyrin micro/nanofiber structures by ionic self-assembly // Materials letters. ISSN 0167-577X. Vol. 164 (2016), p. 160-164.

86. Morkūnė, R.; Lesutienė, J.; Barisevičiūtė, R.; Morkūnas, J.; Gasiūnaitė, Z.R. Food sources of wintering piscivorous waterbirds in coastal waters: A triple stable isotope approach for the southeastern Baltic Sea // Estuarine, coastal and shelf science. ISSN 0272-7714. Vol. 171 (2016), p. 41-50.

87. Boppel, S.; Ragauskas, M.; Hajo, A.; Bauer, M.; Lisauskas, A.; Chevtchenko, S.; Rämer, A.; Kašalynas, I.; Valušis, G.; Würfl, H.-J.; Heinrich, W.; Tränkle, G.; Krozer, V.; Roskos, H.G. 0.25-µm GaN teraFETs optimized as THz power detectors and intensity-gradient sensors // IEEE transactions on terahertz science and technology. ISSN 2156-342X. Vol. 6, iss. 2 (2016), p. 348-350.

88. Mordas, G.; Plauškaitė-Šukienė, K.; Prokopčiuk, N.; Dudoitis, V.; Bozzetti, C.; Ulevičius, V. Observation of new particle formation on Curonian Spit located between continental Europe and Scandinavia // Journal of aerosol science. ISSN 0021-8502. Vol. 97 (2016), p. 38-55.

89. Ratas, I.; Pyragas, K. Macroscopic self-oscillations and aging transition in a network of synaptically coupled quadratic integrate-and-fire neurons // Physical review. E, Statistical, nonlinear, and soft matter physics. ISSN 2470-0045. Vol. 94, iss. 3 (2016), p. art. no. 032215 [1-11].

90. Pyragas, V.; Pyragas, K. Act-and-wait time-delayed feedback control of nonautonomous systems // Physical review. E, Statistical, nonlinear, and soft matter physics. ISSN 2470-0045. Vol. 94, iss.1 (2016), p. art. no. 012201 [1-8].

91. Ulčinas, A.; Picco, L.M.; Berry, M.; Hörber, J.K.H.; Miles, J.M. Detection and photothermal actuation of microcantilever oscillations in air and liquid using a modified DVD optical pickup // Sensors and actuators. A, Physical. ISSN 0924-4247. Vol. 248 (2016), p. 6-9.

92. Stankevičiūtė, J.; Kutanovas, S.; Rutkiene, R.; Tauraitė, D.; Striela, R.; Meškys, R. Ketoreductase TpdE from Rhodococcus jostii TMP1: characterization and application in the synthesis of chiral alcohols // PeerJ. ISSN 2167-8359. Vol. 3 (2015), p. art. no. 1387 [1-18].

93. Remeikaitė-Nikienė, N.; Lujanienė, G.; Malejevas, V.; Barisevičiūtė, R.; Žilius, M.; Garnaga-Budrė, G.; Stankevičius, A. Distribution and sources of organic matter in sediments of the south-eastern Baltic Sea // Journal of marine systems. ISSN 0924-7963. Vol. 157 (2016), p. 75-81.

94. Matijošius, T.; Ručinskienė, A.; Selskis, A.; Stalnionis, G.; Leinartas, K.; Asadauskas, S. Friction reduction by nanothin titanium layers on anodized alumina // Surface & coatings technology. ISSN 0257-8972. Vol. 307, pt. A (2016), p. 610-621.

95. Ežerinskis, Ž.; Hou, X.L.; Druteikienė, R.; Puzas, A.; Šapolaitė, J.; Gvozdaitė, R.; Gudelis, A.; Buivydas, Š.; Remeikis, V. Distribution and source of 129I, 239,240Pu, 137Cs in the environment of Lithuania // Journal of environmental radioactivity. ISSN 0265-931X. Vol. 151 (2016), p. 166-173.

96. Rodin, A.; Grishin, M.; Michailovas, A. Picosecond laser with 11 W output power at 1342 nm based on composite multiple doping level Nd:YVO4 crystal // Optics & laser technology. ISSN 0030-3992. Vol. 76 (2016), p. 46-52.

97. Viskontas, K.; Rusteika, N. All-fiber wavelength-tunable picosecond nonlinear reflectivity measurement setup for characterization of semiconductor saturable absorber mirrors // Optical fiber technology. ISSN 1068-5200. Vol. 31 (2016), p. 74-82.

98. Adamonis, J.; Aleknavičius, A.; Michailovas, K.; Balickas, S.; Petrauskienė, V.; Gertus, T.; Michailovas, A. Implementation of a SVWP-based laser beam shaping technique for generation of 100-mJ-level picosecond pulses // Applied optics. ISSN 1559-128X. Vol. 55, iss.28 (2016), p. 8007-8015.

99. Judžentienė, A.; Garjonytė, R.; Būdienė, J. Variability, toxicity, and antioxidant activity of Eupatorium cannabinum (hemp agrimony) essential oils // Pharmaceutical biology. ISSN 1388-0209. Vol. 54, iss. 6 (2016), p. 945-953.

100. Reklaitis, A. Role of the optical pulse repetition rate in the efficiency of terahertz emitters // Optics communications. ISSN 0030-4018. Vol. 371 (2016), p. 221–225.

101. Asadauskas, S.; Kreivaitis, R.; Bikulčius, G.; Griguce-vičienė, A.; Padgurskas, J. Tribological effects of Cu, Fe and Zn nano-particles, suspended in mineral and bio-based oils // Lubrication science. ISSN 0954-0075. Vol. 28, iss. 3 (2016), p. 157-176.

102. Tyshko, A.; Balevičius, S.; Padmanaban, S. An increase of a down-hole nuclear magnetic resonance tool's reliability and accuracy by the cancellation of a multi-module DC/AC converter's output's higher harmonics // IEEE Access. ISSN 2169-3536. Vol. 4 (2016), p. 7912-7920.

103. Varnaitė-Žuravliova, S.; Sankauskaitė, A.; Stygienė, L.; Krauledas, S.; Bekampienė, P.; Milčienė, I. The investigation of barrier and comfort properties of multi-functional coated conductive knitted fabrics // Journal of industrial textiles. ISSN 1528-0837. Vol. 45, iss. 4 (2016), p. 585-610.

104. Stapulionienė, R.; Vaitkus, S.; Vėjelis, S.; Sankauskaitė, A. Investigation of thermal conductivity of natural fibres processed by different mechanical methods // International journal of precision engineering and manufacturing. ISSN 2234-7593. Vol. 17, no. 10 (2016), p. 1371-1381.

105. Plukienė, R.; Plukis, A.; Puzas, A.; Gvozdaitė, R.; Barkauskas, V.; Duškesas, G.; Cizdziel, J.V.; Bussan, D.; Remeikis, V. Actinides input to the dose in the irradiated graphite of RBMK-1500 reactor // Nuclear engineering and design. ISSN 0029-5493. Vol. 300 (2016), p. 530-535.

106. Barkauskas, V.; Plukienė, R.; Plukis, A. Actinide-only and full burn-up credit in criticality assessment of RBMK-1500 spent nuclear fuel storage cask using axial burn-up profile // Nuclear engineering and design. ISSN 0029-5493. Vol. 307 (2016), p. 197-204.