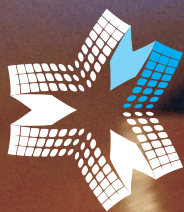
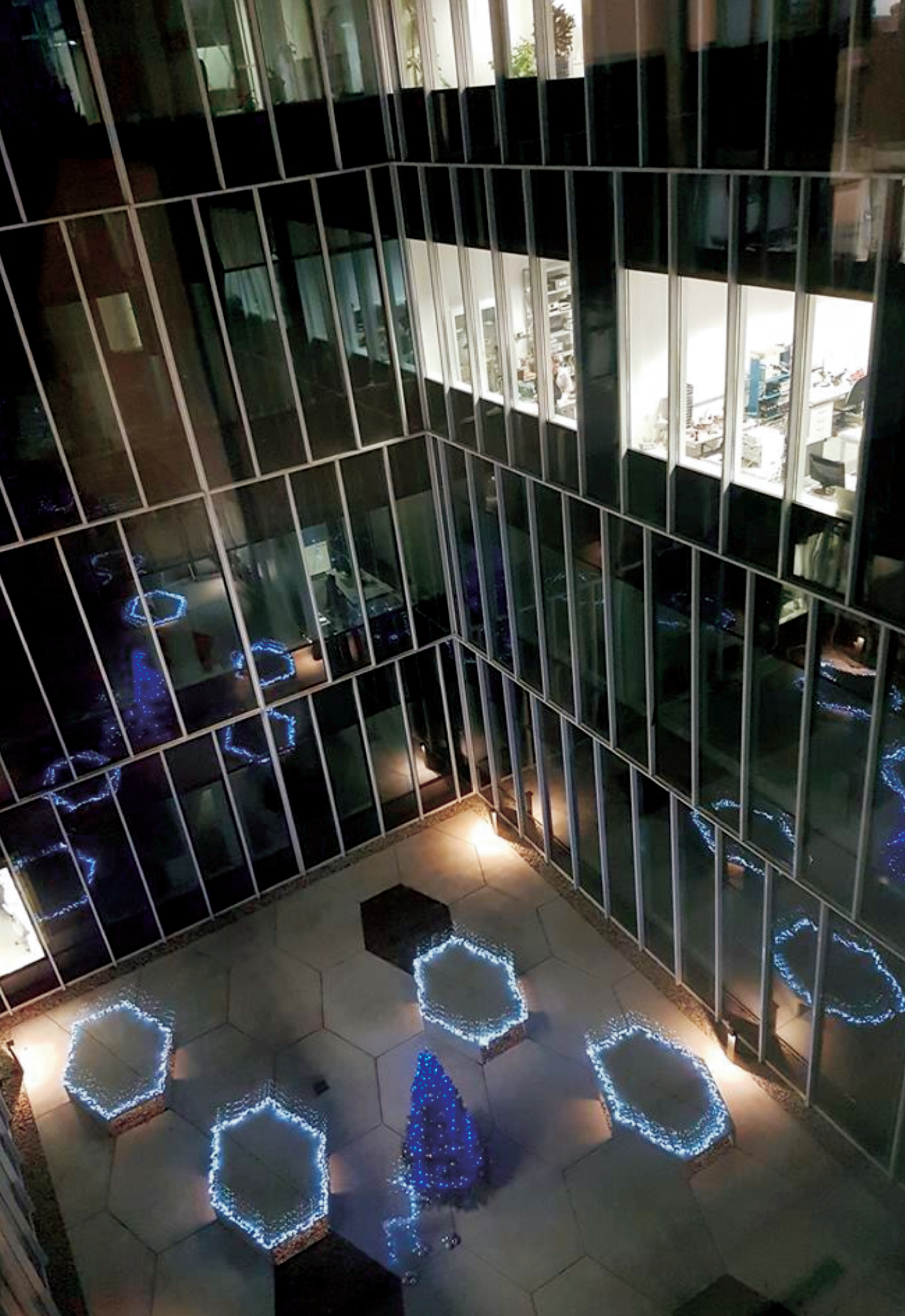


MODERN PATHS TO INNOVATIONS



CENTER
FOR PHYSICAL SCIENCES
AND TECHNOLOGY

ANNUAL REPORT 2018





Message from Director: new dimensions in R&D and capitalization of scientific knowledge

The year of 2018 has been a period of evolution in the Center. The year of 2018 enjoys signatures of fruitful international projects, development of new prototypes and novel technologies, increase in quality and number of scientific publications as well as intensive expansion of innovative services and solutions for international and local industry. The year of 2018 is marked as time for numerous evaluations of the activities in the Center. In addition to the conventional evaluation performed by the Lithuanian Research Council, the Research and Higher Education Monitoring and Analysis Center (MOSTA) organized special Comparative Expert Assessment of Research and Development Activities in all universities and state research institutes. We were delighted to receive positive scores from the experts stating that the absolute majority of units of the Center keep high international level in science, carry out R&D activities exceeding the frame of academic community and display a potential to improve our achievements. The Unit of Photonics and Applied Physics was ranked among the best units in the country.

The year of 2018 has been a period of reconsideration of the mission and vision of the Center:

Center for Physical Sciences and Technology (FTMC) is an institution that focuses on **generation and capitalization of scientific knowledge** in applied physics, chemistry, and technological sciences promoting thus the evolution of high-tech industry.

We are one of the largest fundamental and applied research institutions in **Northern and Central Europe**. It is a globally **competitive place for the research** in the field of physical sciences and technology. We stimulate creativity and culture that **embrace discovery** and **encourage breakthrough innovations**. The key to success is an **atmosphere of cooperation, modern research facilities and attractive career opportunities**.

We rely on our values – Scientific excellence (competence and modern facilities); Versatility and flexibility; Broad, but balanced spectrum of basic and applied research; Knowledge and mind; Effectiveness and networking. We are sure that it will bring us to success in reaching our ambitious aims.

This Annual Report is a traditional illustrated catalogue of important events and enlightening achievements. A survey of most important events that took place in our Departments in 2018 is described in pages that begin here. On-line changes and trailblazing development can be tracked using the barcode given below.

Gintaras Valušis
Director of the Center











APROPÓS 16
ADVANCED PROPERTIES AND PROCESSES IN OPTOELECTRONIC MATERIALS AND SYSTEMS
10-12 OCTOBER, 2018





Fizinių ir technologijos mokslų centras (FTMC) Center for Physical Sciences and Technology

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Laser technologies



Optical coatings, solid-state and fibre 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 a significant part of the photonics related activities, ranging from newly discovered optical 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 the spectral and temporal properties of the light. New laser sources, which are based on tiny but smart fibres or active bulk crystals and are under development in the Fiber Laser and Solid-State Laser Laboratories, provide not only new wavelengths of coherent radiation but high peak power, ultra-short pulses and controlled wavefront as well. Combining of the coherent beams makes the lasers even more powerful. Efficient surface texturing utilising laser beam interference, glass processing utilising smart pulsed lasers or distorted Bessel beams, nano-textures decorated by nanoparticles, 3D metal sculpturing by subtractive and additive technologies, laser-induced transformations in graphene-like materials make up the main working topics of the Laboratories of Laser Microfabrication Technologies. The scope in the 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. Significant progress was made in the validation of novel processes for electroless plating of laser-modified polymers and glasses. 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 microring resonators with the environment. That allows constructing sensitive tools for sensing applications. A large group of scientists, PhD students and engineers work together in laser-related fields. The Department keeps close collaboration with colleagues from other departments of FTMC (Optoelectronics, Physical Technologies, Nanoengineering, Organic Chemistry, Catalysis, Electrochemical Material Science, Characterization of Material Structure) gaining new ideas for joint projects and applications. The year 2018 was again extremely fruitful for the Department of Laser Technologies with plenty of scientific publications in high-ranked peer-review journals.



Laser interference ablation of Si using pulsed lasers

An analytical method for evaluation of thermal diffusion influence to the quality of structures, formed during the laser interference ablation in silicon using femto-, pico-, and nanosecond pulses, was developed. The temperature modulation depth was introduced as a parameter for quality assessment of the laser processing. Based on experimental and simulation data, a new semi-empirical formula, which combines the interference period with the laser pulse duration, the thermal modulation depth and the thermal diffusivity of the material, was derived. The model was used for optimising process parameters in periodical structuring with the required resolution and quality.

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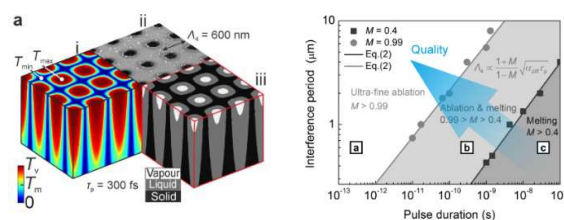


Fig. 1. (left) Thermal field modelling of laser interference ablation: simulated periodical thermal field (i), experimental SEM micrograph (ii) and calculated phase diagram (iii) of silicon just after the absorbance of a laser pulse. Pulse duration: 300 fs. The interference period is $L_4 = 600$ nm. (right) Ablation quality as a function of interference period and pulse duration.

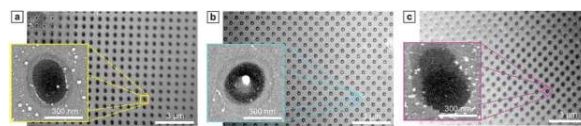


Fig. 2. SEM images of laser interference ablation of Si with various pulse durations: (a) 300 fs, (b) 300 ps, (c) 35 ns.

Efficient material removal using ultra-short pulse lasers

The efficiency of the material removal rate using ultra-short pulse lasers is a limiting factor for their broader application. Numerous process parameters including the scanning speed, the distance between scanned lines, and the spot size should be optimised. A new model of rectangular cavity ablation was developed, considering the decrease in the ablation threshold, as well as saturation of the ablation depth with an increasing number of pulses per spot. Scanning electron microscopy and the stylus profilometry were employed to characterise the ablated depth and evaluate the material removal rate. The numerical modelling showed a good agreement with the experimental results. High speed mimicking of bio-inspired functional surfaces by laser irradiation has been demonstrated.

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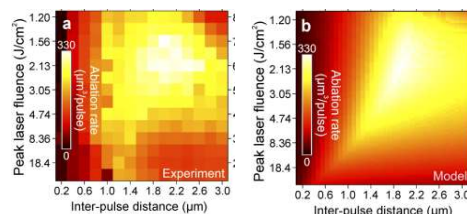


Fig. 3. Laser ablation rate (colour scale) of Cu as a function of the peak laser fluence and inter-pulse distance: (a) experiment, (b) simulation based on the ablation model.

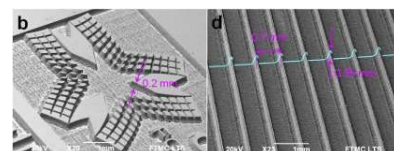


Fig. 4. SEM images of efficient surface structuring by picosecond laser in Cu.

Aberration-controlled Bessel beam processing of glass

The possibility to optimise the glass dicing process by controlling the axicon-generated Bessel beam ellipticity was demonstrated. The ellipticity of the Bessel beam is essential for the glass dicing process. The oblate tip and an elliptical cross-section of a non-ideal (real) axicon results in the non-axisymmetric Bessel beam intensity distribution, which generates intra-volume modifications in the bulk of glass with transverse crack propagation in dominant direction. These distortions could be compensated by the tilt of the axicon perpendicular to its optical axis. The orientation of these modifications parallel to the dicing direction gives significant advantages regarding the processing speed, glass breaking force and cutting quality.

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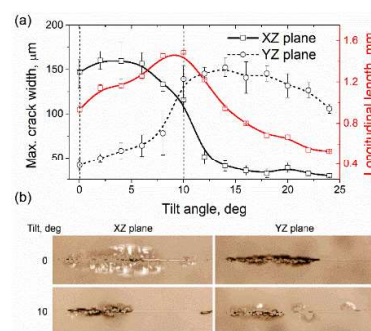


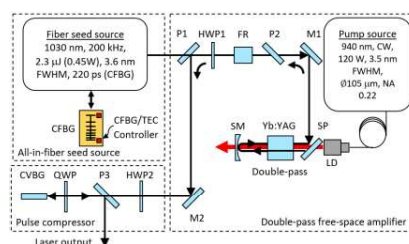
Fig. 5. (a) Laser-induced modification behaviour versus axicon tilt angle, and (b) side view of the Bessel beam induced single-shot modifications in glass at XZ and YZ observation planes for various axicon tilt angles. Beam propagation direction was from left to right.



Compact 20 W femtosecond laser system

We presented a compact femtosecond laser system based on Yb doped fibre seed laser and efficient Yb:YAG crystal rod power amplifier (right Fig.). Matched pair of chirped fibre Bragg grating stretcher and chirped volume Bragg grating compressor was used to obtain high fidelity (Strehl ratio 76%, pulses of 764 fs duration, 104 μ J energy at 200 kHz repetition rate at the output of the laser system). The key novelty of the system was the application of CFBG stretcher and CVBG compressor with matched dispersion which enabled to obtain nearly bandwidth-limited compressed sub-picosecond pulses.

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Development of fibre pulse generators based on non-linear spectral re-shaping

Comprehensive research was carried out to study the operation of the linear fibre pulse generator scheme, based on self-phase modulation-induced spectral broadening and offset-alternating spectral filtering. The influence of the fibre chromatic dispersion and other parameters of the optical scheme for stable pulse generation and the characteristics of generated pulses was described by a numerical model and confirmed by experiments. Self-starting pulse generation was shown experimentally, and the conditions for the achievement of self-starting were found. Results of this research can have a significant impact on the development of novel and reliable ultrashort pulse fibre laser sources.

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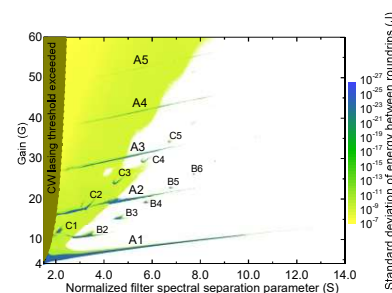


Fig. 6. Simulation results of the pulse generator operation. The standard deviation of the pulse energy (colour) as a function of the gain (G) and normalised spectral separation of the filters (S). Blue area - stable pulse generation, green/yellow – unstable pulse generation, white – no pulse generation.

From fundamental toward applied SERS: shared principles and divergent approaches

Surface-enhanced Raman spectroscopy (SERS) attracts considerable attention as a research tool in surface science. It is also valued for potential applications in analytical sensing. The review of fabrication, properties and operational principles of enhancing substrates is provided in the context of specific application requirements. The performance and utility of the top-down lithographic fabrication, as well as ever more simple and scalable self-assembly techniques, are contrasted and appraised by highlighting selected examples, such as metal-sputtered random template-based substrates of black CuO coated with Au.

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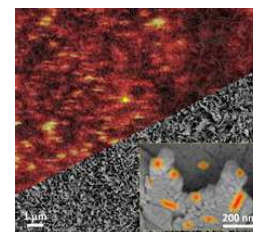


Fig. 7. Stochastic distribution of the SERS-active hot spots on a CuO template-based nanotextured surface coated with 250 nm of Au (top) and SEM image (bottom) of CuO surface. The inset displays a mapping plot of the Raman peak intensity at 1000 cm^{-1} corresponding to the in-plane benzene ring-breathing mode of thiophenol.

Formation of ultrathin metal layers and their application to the metal-dielectric optical elements

Ultra-thin metal films are increasingly applied as functional optical coatings. Various stages of noble metal film deposition were spectroscopically analysed in-situ and ex-situ and compared with modelled characteristics. As a demonstrator, the broad-angle non-polarizing beam splitter with an ultrathin metal layer, combined with dielectric films, was designed, prepared and characterised. It was shown that magnetron sputtering is a suitable technology for fabrication of this kind of optics in a single process.

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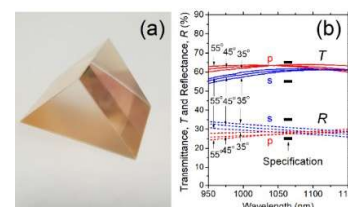


Fig. 8. Non-polarizing beam splitter: (a) picture of a prism with the non-polarizing metal-dielectric coating, (b) its transmittance and reflectance spectra for s- and p-polarised light.

Graphene oxide-dye nanocomposites: effect of molecular structure on the quality of laser-induced graphene

The nanocomposite films made using graphene oxide (GO) and six different organic dyes were employed to produce the laser-induced graphene (LIG) coatings by using near-infrared picosecond laser irradiation. The results of FTIR spectra demonstrated that the GO and dye molecules interact via nitrogen atoms. The Raman spectra have shown that the best quality LIG coating is obtained using a GO-neutral red nanocomposite precursor. A correlation between contact angle, Raman spectra and topological indices of dye molecules was found, and it might be useful for further investigation of the mechanism of LIG production and development of low-defect coatings.

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Plasma etching of substrates for high power laser optics

An efficient method of plasma treatment of polished fused silica (FS) substrates before the coating process was developed for high-power UV-laser optical components. Oxygen plasma of selected energy was chosen to etch the depth of 218 ± 8 nm. This allowed increasing the optical resistance of FS substrates to 75 ± 4 J/cm², which is close to the bulk value. No additional surface roughness degradation was registered after the plasma treatment. The application of etched FS substrates for making anti-reflective (AR) coated components for $\lambda=355$ nm wavelength increased the laser-induced damage threshold (LIDT) by 3.4 times, up to 14 ± 0.7 J/cm² (AR-coated element made on non-etched FS substrate demonstrated just 4 ± 0.2 J/cm²). The large LIDT improvement clearly shows good perspectives to apply the low-energy oxygen plasma etching for producing high-power transparent UV laser optical components.

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High-density gas capillary nozzles manufactured by hybrid 3D laser machining technique from fused silica

The enhanced interest in advanced X-ray sources, driven by laser-accelerated electrons, for the spectroscopic absorption measurement at modest scale research facilities and the demand of higher X-ray energy for the investigation of the warm dense matter, raise the requirement of manufacturing and characterisation of tailored gas targets with micrometric dimensions. In this report, an efficient hybrid laser technique, nanosecond laser rear-side processing and femtosecond laser-assisted selective etching (FLSE) for the manufacturing of high-density gas capillary targets, is demonstrated. Cylindrical capillary nozzles for laser betatron X-ray sources were numerically simulated, manufactured from fused silica by 3D laser inscription and characterised using interferometry and gas density reconstruction.

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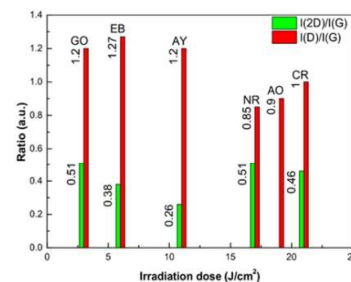


Fig. 9. The ratio of the Raman spectra line intensities I_{2D}/I_G and I_D/I_G in GO and GO-dye composites after laser treatment at the highest reduction level. Numbers correspond to the used laser irradiation doses in J/cm².

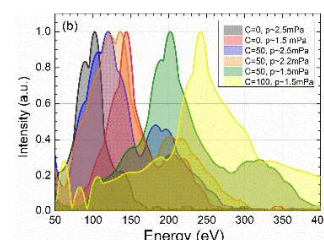


Fig. 10. Energy spectra of oxygen plasma depending on process parameters.

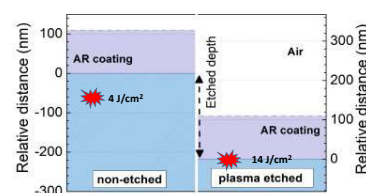


Fig. 11. Relative distances of damage sites for AR-coated non-etched and etched FS substrates. The coating and substrate interface was selected as a zero level.

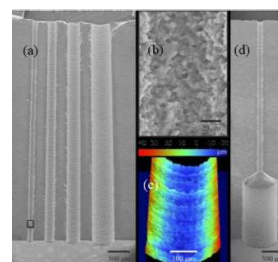


Fig. 12. (a) SEM images of a cross-section of drilled holes with diameters of 100 μm , 200 μm , 300 μm and 500 μm ; (b) the magnified image of the 100 μm -diameter channel surface; (c) the surface topography of 500 μm -diameter channel, and (d) the 100 μm -diameter capillary connected with a 0.8 mm-diameter adapter.

Optoelectronics



PhD students of the Department (from left-to-right): Ignas Nevinskas, Ričardas Norkus, Vytautas Janonis, Domas Jokubauskis, Justinas Jorudas, Ieva Belickaitė, Andrius Rimkus, Simona Pūkienė, Sandra Stanionytė, Evelina Pozingytė

Optoelectronics is widely recognised as one of the Key Enabling Technologies

The research of Optoelectronics Department can be distinguished in two main directions: (i) epitaxial growth technology of semiconductor nanostructures and development of devices for mid- and far-infrared spectral ranges and (ii) Terahertz (THz) imaging and spectroscopy, its applications and development of compact THz photonics components and systems. Moreover, the Department operates a comprehensive set of standard optical characterisation techniques that are intensely exploited also by other Lithuanian research groups and high-tech companies. Terahertz (THz) radiation, which lies in the frequency gap between the infrared and microwaves, referred to as the frequencies from 100 GHz to 30 THz, has long been studied in fields such as astronomy and analytical science. 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 commercialised by two companies that have been started by the researchers of the Department. During the year under reference, the researchers of the Department investigated the physical origin of THz emission from the surfaces of various semiconductors illuminated by femtosecond laser pulses. It has been demonstrated that this emission from narrow gap semiconductors such as InAs or InSb, which are most efficient THz emitters at the moment, is caused by the electron energy bandgap anisotropy and lateral photocurrents appearing due to this anisotropy. Moreover, the ultrafast measurement facilities of the Department are becoming increasingly attractive for the scientist from abroad, performing their investigations in Vilnius. Scientific research activities are supported by the Research Council of Lithuania and the European Space Agency; the Department intensively cooperates with high tech companies in Lithuania and abroad.



Terahertz imaging for security applications

Fibonacci or bifocal terahertz (THz) imaging is demonstrated experimentally employing a silicon diffractive zone plate in a continuous wave regime. Images simultaneously recorded in two different planes are exhibited at 0.6 THz frequency with a wavelength limited spatial resolution. Multi-focus imaging operation of the Fibonacci lens is compared with a performance of the conventional Fresnel zone plate. Since both planes are in focus of the Fibonacci lens, all the objects including pencil-written letters “FTMC” are clearly resolved in a single shot.

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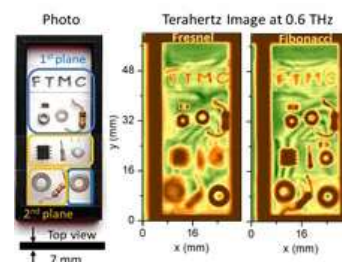


Fig 1. Photo of the objects (left) placed at two image planes separated by 7 mm and terahertz image pictured with the Fresnel (center) and Fibonacci (right) lens.

Non-destructive inspection of food and technical oils by terahertz spectroscopy

Terahertz spectroscopy was used to monitor pure and degraded oils as well as hydrocarbon chemicals. Significant differences in the terahertz properties arising from the presence of ester linkages in the edible and technical oils were obtained. The explicit increase of the refractive index (RI) in all THz spectrum range was observed in hydrocarbons and mono-functional esters with the increase of molar mass, in contrast to RI dependence on molar mass in multi-functional esters, such as adipate or vegetable oils. Degradation products, oleic acid and water, in particular, lead to some changes in absorption coefficient and the refractive index of vegetable oils monitored by a non-uniform dependence of terahertz properties on the extent of degradation.

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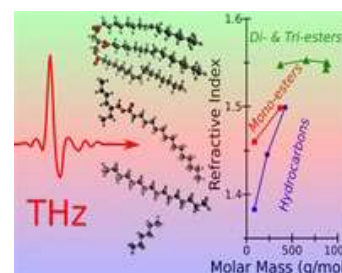


Fig. 2. Measurement of the RI in all THz spectrum helps to identify the hydrocarbons and mono-functional esters and monitor their molar mass.

Semiconductor energy band structure investigated by THz excitation spectroscopy

After excitation by femtosecond laser, all semiconductor materials emit pulses of THz radiation. This occurs because photo-excited electrons move ballistically away from the surface leaving less mobile holes behind, creating a dynamically changing electrical dipole. By changing the laser photon energy and monitoring the radiated THz pulses, the details of the band structure at different electron energies (such as the bandgap, the separation between different conduction band minima, the heterostructure band offsets, etc.) can be determined.

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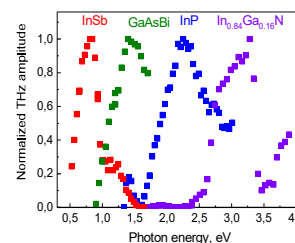


Fig. 3. The THz excitation spectra of various semiconductors used for determining energy band structure parameters: the G-L intervalley energy separation in InSb and InP, the G-L and G-X separations in GaAsBi with 9%Bi and the band offsets in InGaN/GaN heterostructure.

THz-excitation spectroscopy technique for band-offset determination

The experimental THz-excitation spectroscopy technique for a determination of heterojunction band offsets is suggested. When photoexcited electrons gain sufficient energy to pass the potential barrier ΔE_c , corresponding to a conduction band offset, an amplitude of THz-emission pulse sharply increases, making it possible to measure the offset value directly. The technique is applied for a determination of GaAsBi-GaAs band offsets. The deduced conduction band offset of GaAsBi-GaAs heterojunction is of about 45% of an energy gap difference.

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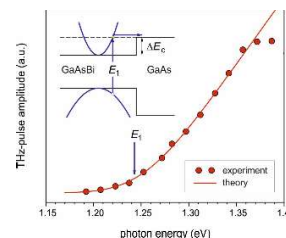
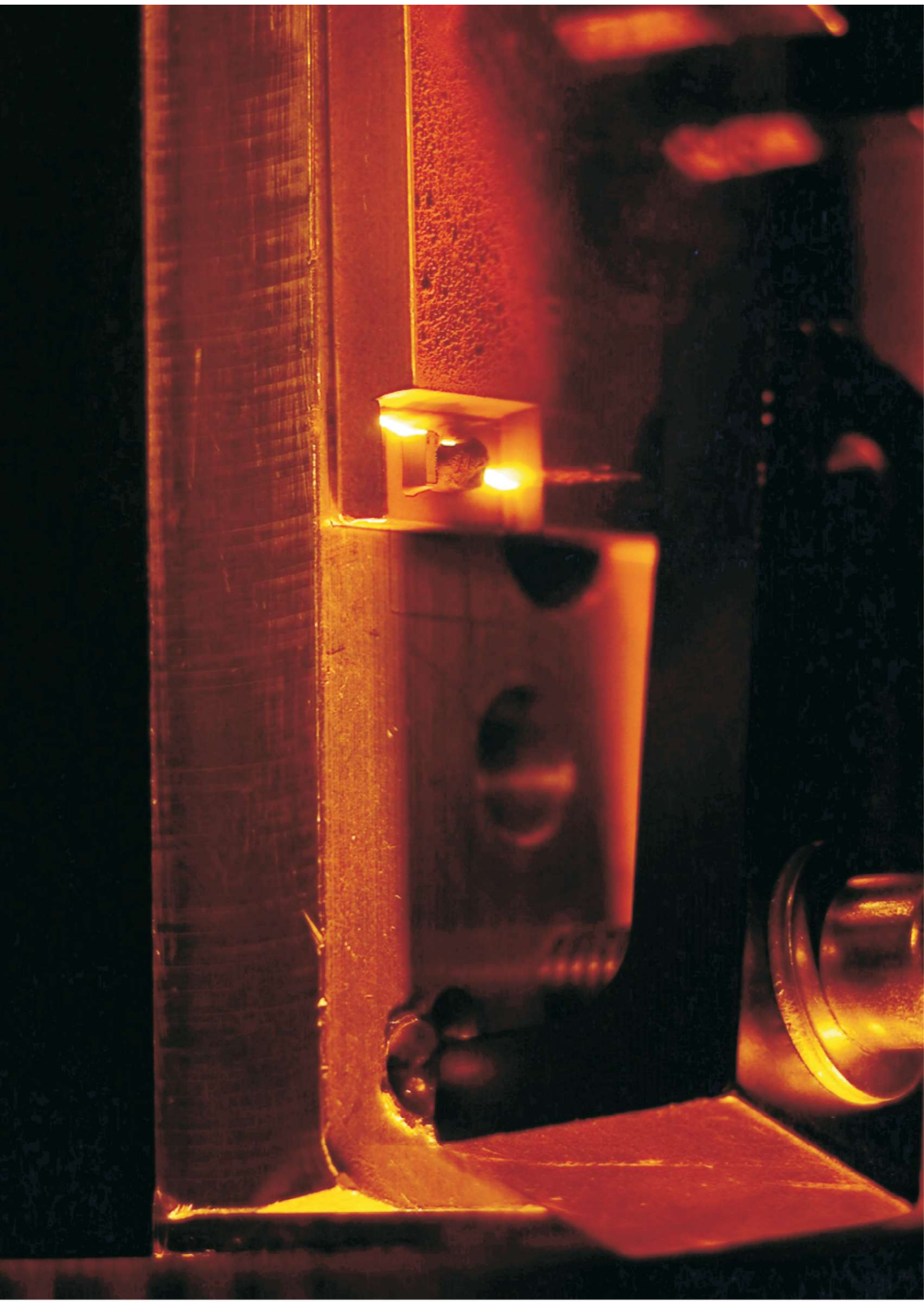
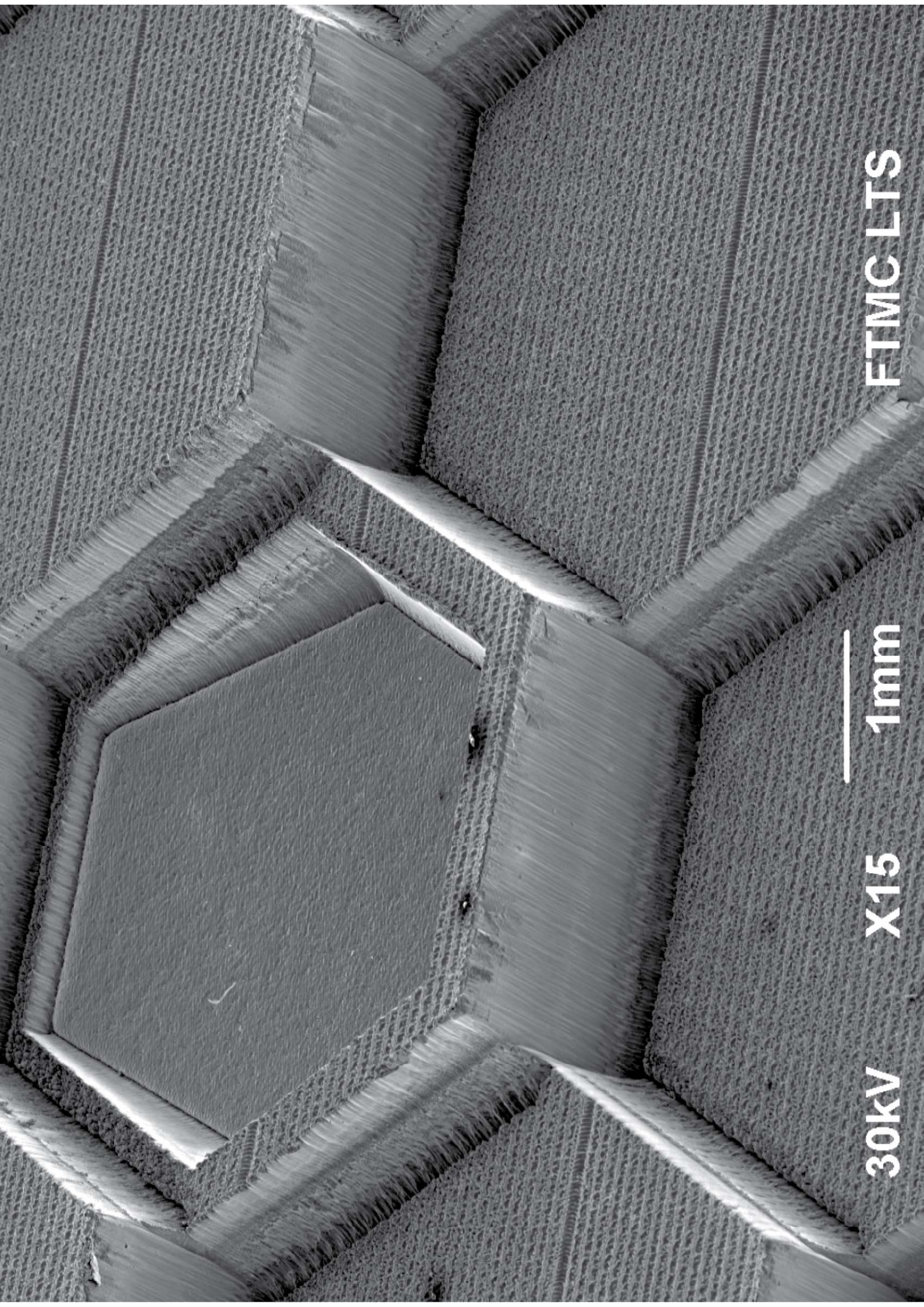


Fig. 4. The THz-pulse excitation spectrum of GaAsBi-GaAs heterostructure. The THz pulse is emitted when the electron excess energy is sufficient to overcome the potential barrier ΔE_c .





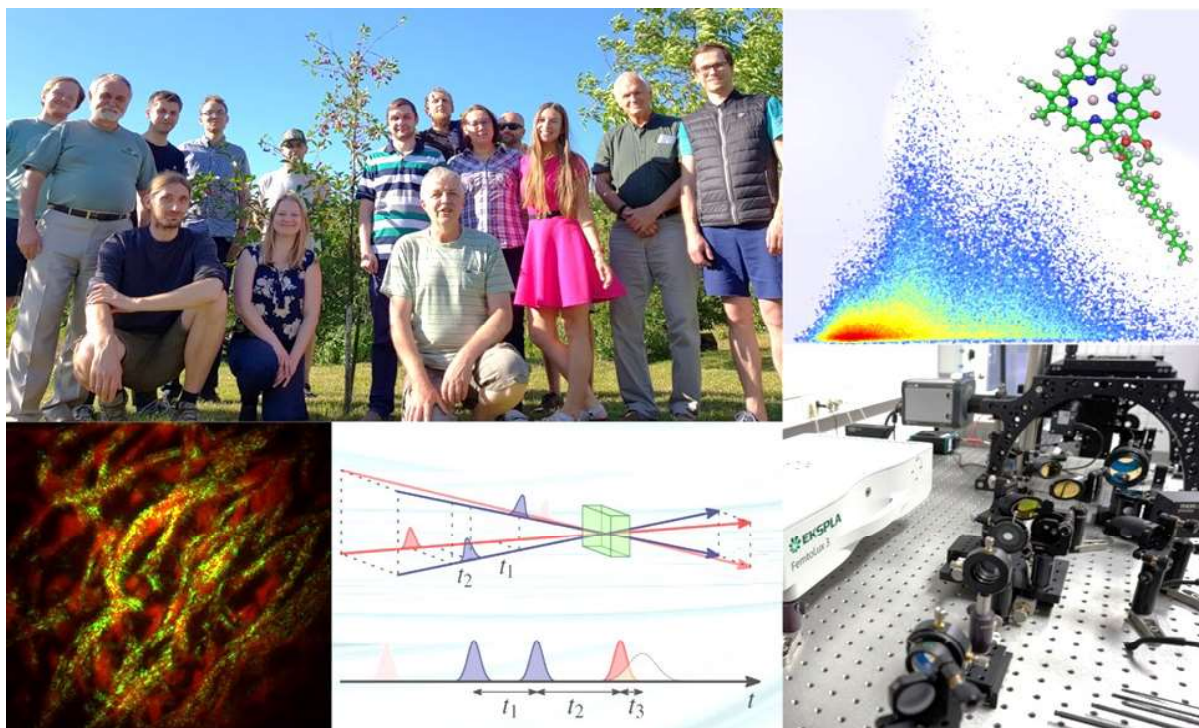
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Molecular physics and nanoengineering



Excitation dynamics and dissipation in natural and artificial molecular systems

Molecular systems, mostly studied 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 dominated entirely 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, applications require 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 human-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, 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 accounted for 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 utilised by Nature to select and optimise 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.



Oxide allows enhancing photocurrent gain in the perovskite photodetectors by order of magnitude

Planar photoresistor-type perovskite photodetectors show high sensitivity, which is enhanced by the current multiplication effect: photogenerated charge carrier initiates injection and passage of several additional electrons or holes. We investigated the influence of a naturally formed or artificially deposited metal oxide layer on the electrodes of a hybrid-perovskite photodetector on its sensitivity governed by photocurrent multiplication. It was demonstrated that the oxide layer enhances sensitivity by order of magnitude by hampering the extraction of photogenerated holes, which accumulate in energetic traps near the negative electrode and reduce the barrier for the electron injection. This enables to make a photodetector with one of the highest currently reported responsivities just by simple one-step deposition of the perovskite layer from the solution onto interdigitated Cr electrodes with a naturally formed CrO_x layer. Such a simple method of enhancing photodetector sensitivity together with the provided photocurrent gain mechanism may open new opportunities for the development of cheap and easily producible planar perovskite photodetectors.

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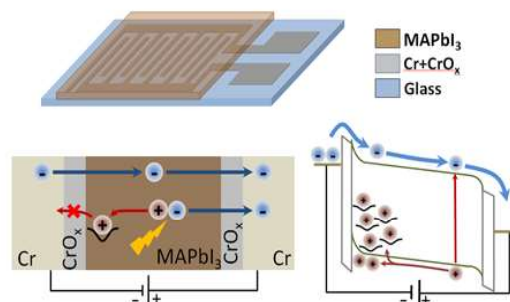


Fig. 1. The device structure of the plain polycrystalline perovskite photodetector fabricated on interdigitated comb electrodes. The chromium oxide layer on interdigitated electrodes enhances its performance. The space charge field of the trapped holes lowers the barrier height for electron injection, thus enhancing photocurrent gain by order of magnitude. Perovskite deposited on chromium oxide-based electrodes shows around 360-fold photocurrent enhancement and about 5 ms response time.

Oxidative state of photosystem II reaction center controls the level of photoprotection in plants

Photosystem II (PSII) of higher plants is protected against light damage by thermal dissipation of excess excitation energy, a process that can be monitored through non-photochemical quenching (NPQ) of chlorophyll fluorescence. When the light intensity is lowered, non-photochemical quenching largely disappears on a time scale ranging from tens of seconds to many minutes. With the use of picosecond fluorescence (FL) spectroscopy, we demonstrated that one of the underlying mechanisms is only functional when the reaction centre of PSII is closed, that is when electron transfer is blocked, and the risk of photodamage is high. This is accompanied by the appearance of a long-wavelength FL band. As soon as the reaction centre reopens, this quenching, together with the long-wavelength fluorescence, disappears instantaneously. This allows plants to maintain a high level of photosynthetic efficiency even in dangerous high-light conditions.

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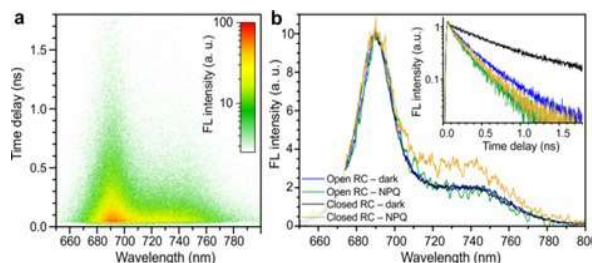


Fig. 2. Picosecond fluorescence spectroscopy on spinach leaves subjected to different excitation conditions. (a) The measured time-resolved fluorescence from dark-adapted spinach leaves with open reaction centers (RCs). (b) Steady-state fluorescence spectra and kinetics (inset) of photosystem II under various conditions, as obtained by decomposing the experimental data into two components (PSI and PSII). Further analysis revealed that the appearance of the far-red FL band in the light-adapted PSII with the closed RCs is accompanied with the higher NPQ yield, compared to the same conditions with the open RCs.



Dynamics of charge distribution in sandwich-type light-emitting electrochemical cells revealed by the Stark effect

A sandwich-type structure composed of thin films of functional materials is the dominant architecture of organic optoelectronic devices. During the device operation, injected or inside generated electrical charges arrange in a specific spatial distribution. This distribution affects the electric field profile throughout the layers and has a fundamental impact on charge transport and recombination/separation processes. However, probing of the charge distribution is challenging because the hidden active layers are experimentally not directly accessible. We study the organic light-emitting electrochemical cells (LEC) and demonstrate that electroabsorption spectroscopy in combination with electrical capacitance measurements enables the determination of the distribution of the injected, uncompensated electronic charge inside these devices. Under constant-voltage operating conditions, the Stark effect signal intensity and the capacitance increase steadily, but to a different extent. We demonstrate that this difference sensitively depends on the position and distribution width of injected mobile electrons. Estimates show a substantial spreading over the active layer of the injected electron density with time, screening the electric field behind the charge peak.

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A twisted tale: measuring viscosity and temperature of microenvironments using molecular rotors

Measuring viscosity and temperature on the microscale is a challenging yet essential task, in materials sciences and biology alike. Here, we have reviewed and discussed fluorescent microviscosity sensors, termed 'molecular rotors', that offer a convenient way of measuring microscopic viscosity and sometimes may even be used to measure microscopic temperature in addition to viscosity. We have discussed how temperature in combination with various solvent properties can affect microviscosity measurements, and we have reviewed possible action mechanisms that make molecular rotors sensitive to multiple parameters of their environment. Overall, we have revealed a complicated, yet exciting, behaviour of molecular rotors at different viscosity, temperature and solvent properties on the microscale and how this behaviour can be explained and exploited.

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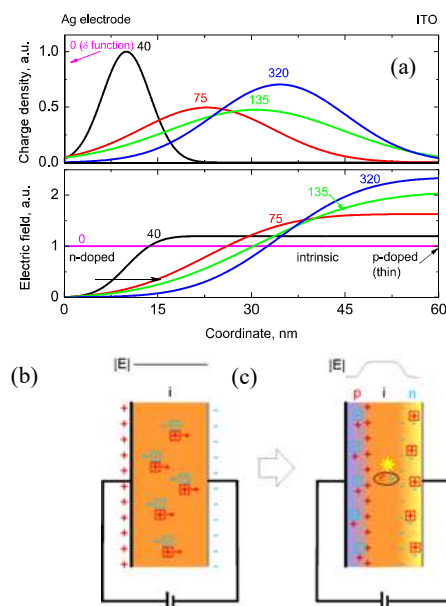


Fig. 3. (a) Gaussian distributions of the uncompensated electron charge densities and electric fields at different operation times (min) for a 60 nm thick cyanine Cy3P LEC operated at 4 V. The p-doped zone is assumed to be very thin and not growing over time. (b) The cross-section of LEC device upon application of the bias, squares indicate the moving ions. (c) The formation of the p- and n-doped zones inside the LEC, distinctive distribution of the charges and the electric field.

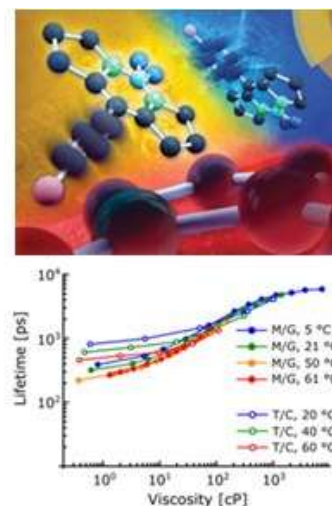


Fig. 4. Viscosity, temperature and polarity sensitivity of molecular rotor BODIPY-C₁₀. Fluorescence lifetimes of the rotors measured in methanol-glycerol (filled circles) and toluene-Castor oil (empty circles) mixtures of varying viscosity and varying temperature.

Fluorescence quenching based evaluation of glucose oxidase composite with polypyrrole

Glucose oxidase composites with conducting polymers (e.g. polypyrrole) is an excellent nano-biomaterial suitable for the design of bioelectronic devices such as biosensors and biofuel cells. The exploration of native GOx and flavin adenine dinucleotide (FAD) solutions confirmed that about 5% of FAD dissociated from GOx during the period of solution preparation and this fraction remains constant within one month. It was found that polypyrrole, which formed composites with FAD and GOx, facilitated the removal of FAD molecules from GOx and twice reduced the fluorescence decay rate. It was found that the polypyrrole and FAD composite with polypyrrole effectively quenched the FAD fluorescence, and FAD could not freely unfold. The findings are beneficial in the selection and adaptation of enzyme immobilisation strategies, which are applied in the development of biosensors and biofuel cells.

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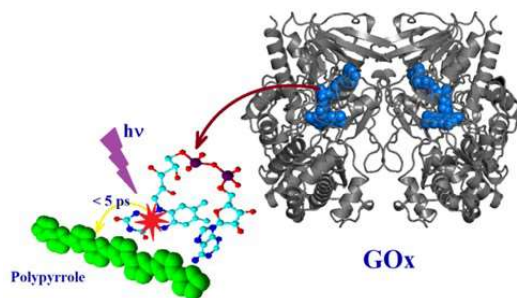


Fig. 5. Schematic representation of withdrawing of all FAD molecules from the GOx complex by polypyrrole oligomer. Polypyrrole effectively quenched the FAD fluorescence and did not allow FAD to unfold.

Single-liposome fluorescence microscopy reveals LHCII proteoliposome heterogeneities

A novel strategy employing methods of proteoliposome preparation, fluorescent labelling, purification, and surface immobilisation allowed quantifying various properties of the proteoliposome sample using fluorescence microscopy at the single-liposome level. This strategy was for the first time applied to study proteoliposome sample with photosynthetic pigment-protein complexes LHCII. We showed that LHCII proteoliposome samples, even after purification with a density gradient, always contain a fraction of non-reconstituted protein and are incredibly heterogeneous in both protein density and liposome sizes. This strategy enables quantitative analysis of the reconstitution efficiency of different protocols and precise fluorescence spectroscopic study of various transmembrane proteins in a controlled native-like environment.

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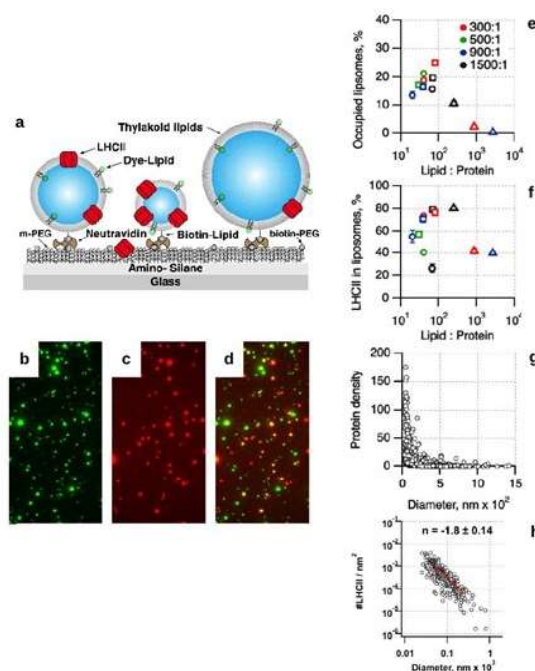


Fig. 6. Fluorescence microscopy of single LHCII proteoliposomes. (a) Proteoliposome immobilisation strategy. (b–d) Micrographs obtained via the (b) liposome ch., (c) LHCII ch., and (d) both ch. overlaid. Percentage of the occupied liposomes (e) and reconstituted LHCII complexes (f) vs lipid/protein ratio of the sample. (g) The relation between the protein density in the proteoliposome and the liposome diameter. (h) Distribution of the LHCII mean surface concentration for liposomes of various sizes.

Toward more realistic biophysical models of the cell membrane

Self-assembled monolayers (SAMs) on solid surfaces are often used as supports for tethered bilayer lipid membranes (tBLMs). Such a platform is advantageous from the application point of view as it allows to precisely control the composition and geometry of different biomimetic assemblies. We have undertaken a systematic, combined experimental and theoretical study on a series of self-assembled monolayers (SAMs) on gold designed for adjustable tethering of model lipid membrane phases. We have employed ellipsometry, contact angle goniometry, and infrared reflection-absorption spectroscopy (IRRAS) and we have characterised the obtained mixed SAMs with variable surface densities of the anchors. We have observed two different scenarios of spatial distributions of the anchoring molecules (Fig. 1). The short anchoring molecules are randomly distributed over the mixed SAM surface and do not segregate even at high surface densities (up to 40 mol %). Contrary, the long anchor partially phase segregates and self-associates on the surface, even at low surface densities of a few mol %. The above described experimental findings were supported and confirmed by molecular dynamics simulations (Fig. 2). Despite the observed structural differences of the mixed SAMs, the recorded quartz crystal microbalance kinetics indicated that small unilamellar vesicles efficiently rupture and form a tBLMs on both types of surfaces. Thus, the developed anchoring SAMs with well-controlled structural characteristics and phase behaviour are suitable for obtaining tBLMs that can be further employed for advanced studies and applications of different cell membrane-mimicking and artificial assemblies, including high-throughput screening.

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Atomic force microscopy characterisation of supramolecular constructs

Tubular nanoscale supramolecular constructs are attractive for applications including transport, flow-through catalysis, separation and detection. Such nanoarchitectures have been developed and characterised in collaboration with scientists from Vilnius University. Recently, we have proposed a new strategy towards the formation of nanotubular hydrogen-bonded polymers based on the self-assembly of isocytosine tautomers in orthogonal directions. Atomic force microscopy (AFM) proved to be suitable for independent verification of formation of the tubular polymeric aggregates and their maintenance on solid surfaces. Such analysis revealed a gel-like fibrous network structure composed of entangled bundles of tubular polymers and provided indirect proof for the gelation mechanism. Based on molecular models, it was possible to identify intact molecular tubes on a solid support. Current efforts of the collaborating groups aim at developing new molecular devices based on the built constructs.

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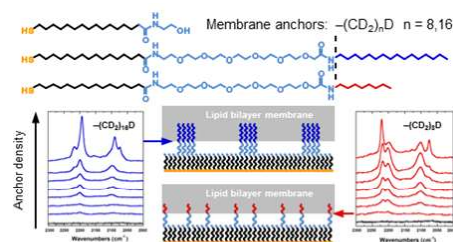


Fig. 1. Chemical structures of the molecular building blocks for the self-assembly of tuneable, nanometer-scale interfacial phases for anchoring of supported lipid bilayers, as explained in the cartoon. FTIR spectra of the C-D stretching region of self-assembled monolayers (SAMs) on gold formed by the above compounds reveal two different types of structures regarding molecular packing of the tail groups in the SAMs.

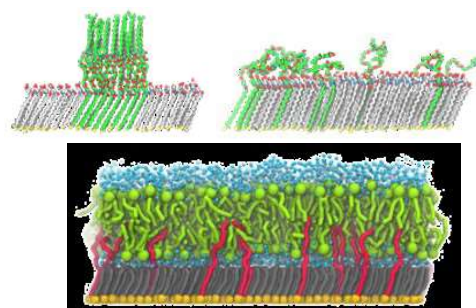


Fig. 2. Top images: Full atomistic molecular dynamics simulations indicate anchor molecule clustering or homogeneous dispersion in the SAM [2], a result in good agreement with the experimental data. Bottom image: simulation of a cell membrane-like assembly obtained on one of the designed anchoring architectures.

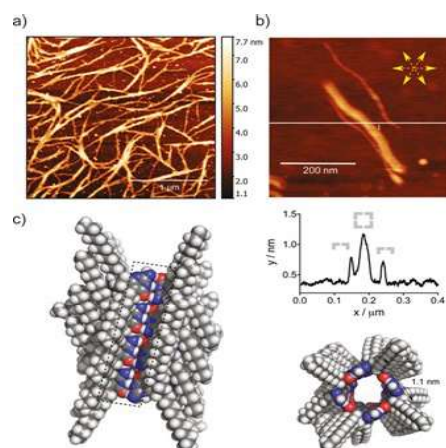
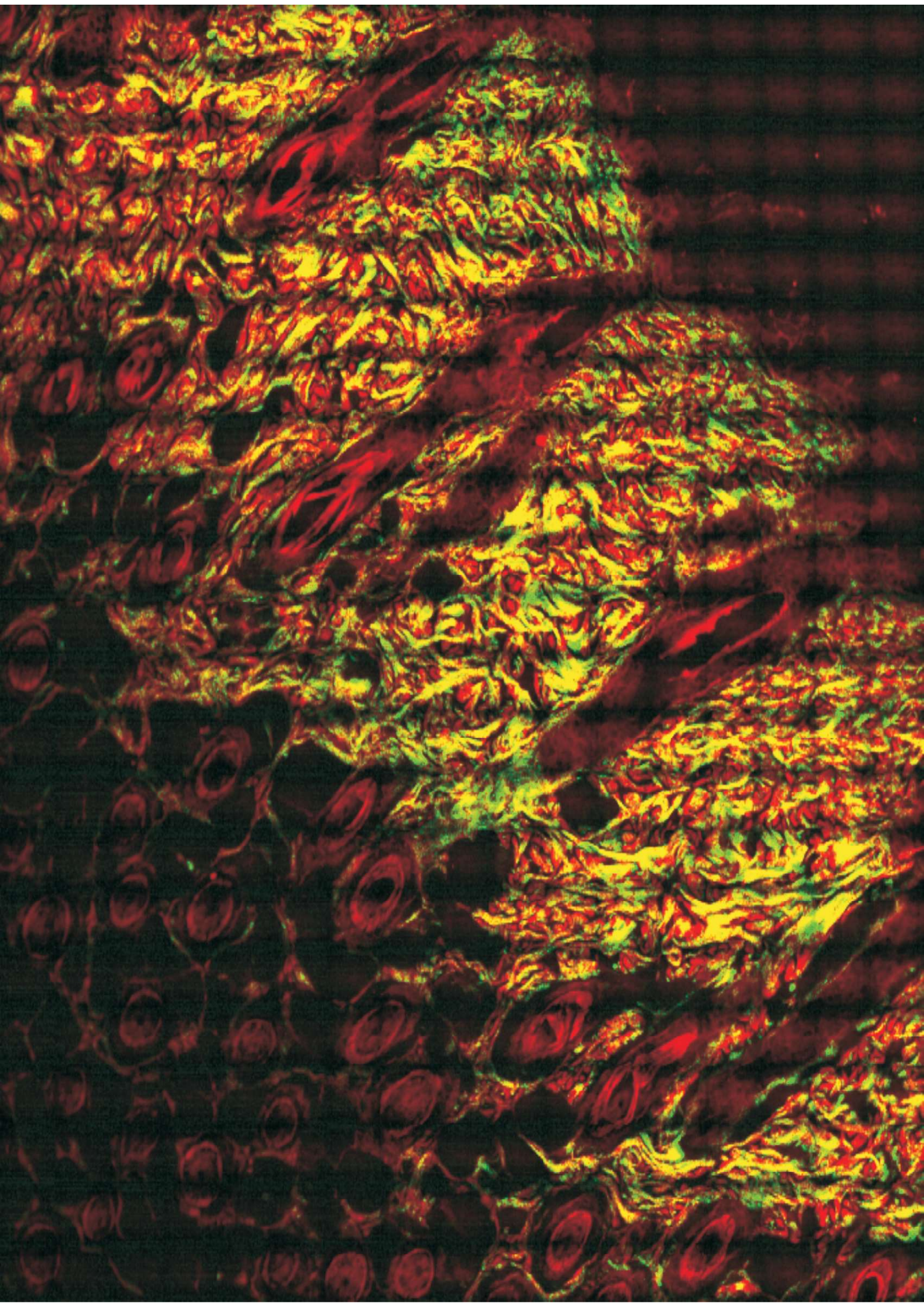
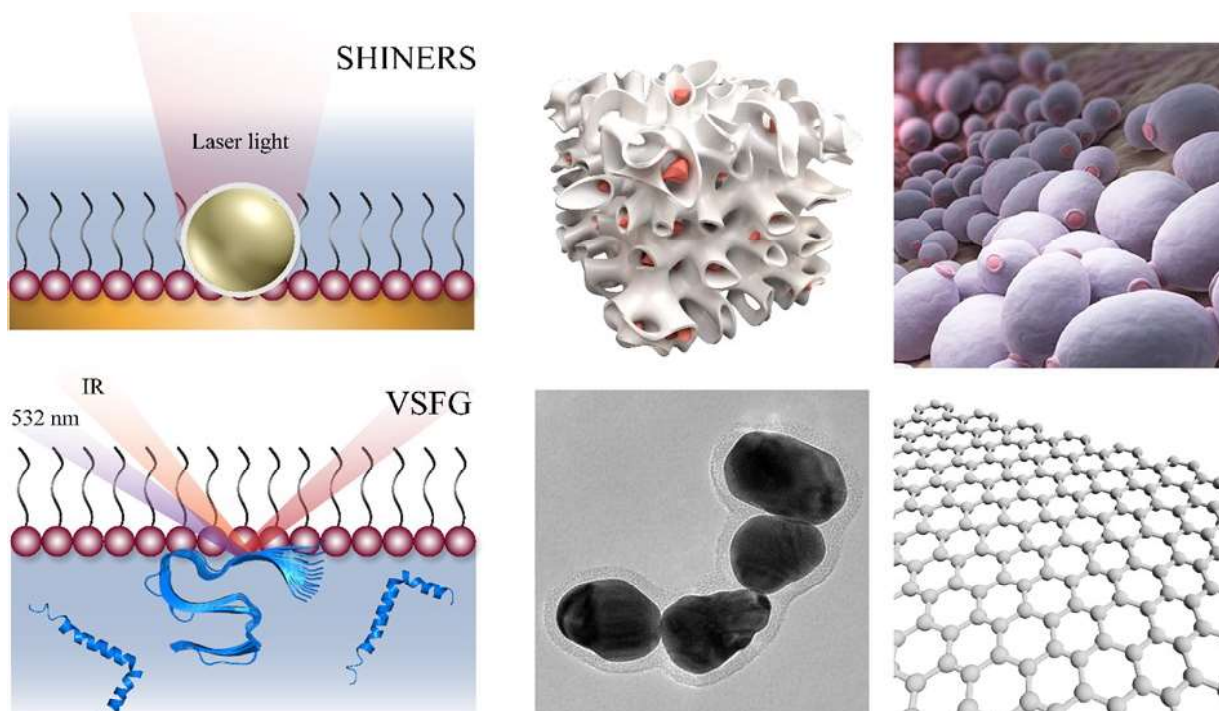


Fig. 3. (a) AFM image of the fibrous network obtained from diluted sol. (b) (top) AFM image of laterally aggregated tubular aggregates; (middle) cross-section profile showing intact and partially collapsed nanotubes; (bottom) top-view of the molecular model of the tubular polymer. (c) Side-view of the molecular model of the tubular polymer.



Spectroelectrochemistry



Cover figures. Top: (left) representation of SHINERS application to study a self-assembled monolayer; (middle) lipid liquid crystalline phase (LLC) with inserted protein (in red) that was studied with Raman spectroscopy; (right) yeast cells. Bottom: (left) representation of VSFG application for protein aggregation study; (middle) TEM image of Au nanoparticles coated with SiO₂; (right) graphene layer.

Spectroscopy of adsorption and biochemical processes at surfaces and interfaces

Electron transfer reactions, electrocatalysis, the functioning of biomolecules, self-assembly, and various biochemical processes take place predominantly at the surfaces and interfaces. To predict and control the way those processes will proceed, a molecular level understanding is required. Our group employs and develops novel spectroscopic techniques that enable to probe complex liquid and solid interfaces that are difficult to study with most common spectroscopic techniques. Shell-isolated nanoparticle-enhanced spectroscopy (SHINERS) is the most promising vibrational surface-enhanced Raman technique. It was developed to overcome the limitations of substrate use in surface-enhanced Raman spectroscopy (Tian et al. 2010). Our group produces a thin silicon dioxide layer coated Au and Ag nanoparticles. The shell layer plays two very important roles: it protects the nanoparticles from degradation and prevents unwanted interactions between nanoparticles and probe molecules. Recently, our group used SHINERS to study potential-induced changes in the molecular structure of self-assembled molecules (more on the next page) and to characterize the surface of functionalized graphene and a biological system of yeast cells. Vibrational sum-frequency generation spectroscopy (VSFG) is a unique technique with an intrinsic surface specificity. It enables to record the vibrational spectrum explicitly of the surface without any interference with a signal from the bulk material. It is a very versatile technique that can be used to study many different surfaces and interfaces such as solid/air, solid/liquid, liquid/air. We applied VSFG to study hole transporting self-assembled monolayer that was formed on a perovskite solar cell (more on the next page). The greatest potential of VSFG lies in its ability to measure liquid surfaces with a sensitivity of a few molecular layers. Currently, we are studying the aggregation of proteins at the surface of model lipid membranes using VSFG. The aim of our study is to answer one of the most important questions in biology and chemistry: what is the role of protein-membrane interaction in the protein aggregation process?

Shell-isolated nanoparticle-enhanced Raman spectroscopy study of the positive charge bearing monolayer

Electrode potential effect on the molecular structure of adsorbed species at an interface is one of the most critical issues in physical electrochemistry. In this study, self-assembled monolayer consisting of N-(6-mercapto)-hexylpyridinium (MHP) was formed on a smooth gold electrode in an aqueous perchlorate solution. Shell-isolated nanoparticle-enhanced Raman spectroscopy (SHINERS) was used to probe the electrochemical potential effect on bonding with the surface, ion-pairing, and molecular structure of MHP monolayer. The results obtained using in situ electrochemical SHINERS demonstrate that the Au–S stretching frequency exhibits near linear blue shift as the electrode potential is tuned to more positive values. The frequency tuning rate was found to be as high as $18.6 \pm 0.9 \text{ cm}^{-1}/\text{V}$. Additionally, the analysis of ion-pairing at interface revealed a decrease in intensity of the vibrational spectrum of electrostatically attracted perchlorate anions at more negative potential values.

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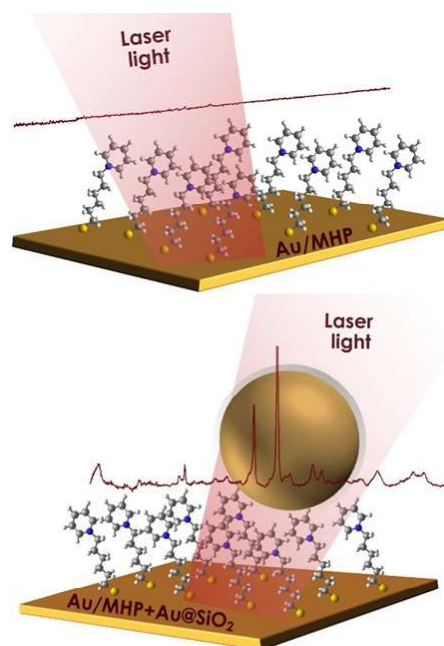


Fig. 1. Comparison of Raman spectrum of MHP adsorbed on smooth Au electrode (Au/MHP) and SHINERS spectrum from smooth Au electrode with adsorbed MHP (Au/MHP + Au@SiO₂).

Self-assembled hole transporting monolayer for highly efficient perovskite solar cells

In this work, a team from HZB (Helmholtz-Zentrum Berlin für Materialien und Energie) and KTU (Kaunas University of Technology) has synthesised a novel molecule (V1036) that self-assembles into a monolayer (SAM), and it was used as an electrical contact layer for perovskite solar cells. This molecule is comprised of several carbazole rings and is functionalized with a phosphonic group via which molecule anchors itself to an oxide substrate and forms a dense and compact monolayer. The SAM and its further modifications were characterised by our group using surface sensitive sum-frequency generation spectroscopy (VSFG) and Fourier transform spectroscopy (FTIR). Vibrational bands that correspond to characteristic vibrations of V1036 were identified, and surface coverage and packing were evaluated as well. Such characterisation was crucial to show that V1036 actually binds to the oxide surface and to link the quality of the SAM with the improvement of the overall efficiency of the perovskite solar cell. For the first time a hole-transporting SAM was used in perovskite-based solar cell, and power efficiency of 17.8% was reached.

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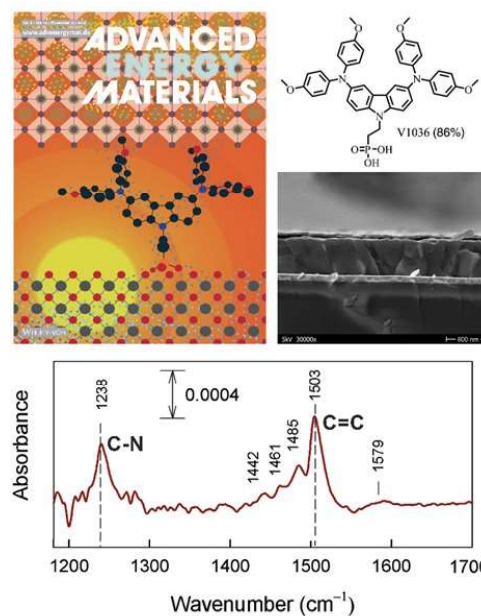


Fig. 2. This study appeared on the front cover of Advanced Energy Materials (HZB/Saule Magomedoviene). Chemical structure of V1036, cross-sectional SEM micrographs of the perovskite film and a characteristic FTIR spectrum of SAM.



Nanostructures for applications



The ultimate aim of our applied research is to develop the sensors and sensor systems acceptable to characterise physical and chemical conditions of the surrounding. In our R&D work, we are trying to create novel techniques for the semiconductor technology adequate to combine the usual thin solid films with the two-dimensional (2D) materials. Our target is a fabrication of the hybrid photonic devices and the functional elements that can be integrated as the key enabling components in the autonomous intelligent systems. Three deeply related parts are considered being the core fields in our work. First, synthesis and investigation of the functional materials and related structures. Second, testing of the novel ideas in the working models of the devices. Third, development and testing of the prototypes of the devices and integrated systems compatible with the intelligent data collection and analysis networks, typically called the Internet of Everything (IoE). Therefore, the combined self-powered systems based on the 2D-materials, ultra-thin layers and epitaxial quantum structures are the core target in our R&D work. These systems can be made on flexible and transparent substrates, thus handy and light. These modules can be easily integrated into small volume devices, small robots, gadgets and even used as the smart dust.

2D material technology for gas and photo-sensitive systems

Our current work is limited to the two types of 2D materials, namely graphene and MoS₂ as a model material of the transient material dichalcogenides (TMDs). The CVD based synthesis, transfer and treatment methods must be understood and adapted to the fabrication of a vertically stacked up multi-layered structures with the 2D materials (graphene, molybdenum disulphide) and ultra-thin films (metal and metal oxides). Since the van der Waals interaction between the stacked layers are known to play an essential role; it is highly important to understand the influence of the intentional treatment on the characteristics of the stacks. In this report, we introduce our investigation of the annealing time effect on the graphene (G) – metal (Au and Ni) stack. Detailed analysis of the Raman spectra similar to that in Fig.1 revealed the mechanisms of the changes in the electrical properties of the stacks. We observed much larger doping effect for the G–Ni stack than for the G–Au. However, the strain effect was dominant in the G–Au stack. Based on the acquired understanding of the interface interactions, we optimised the conditions of the annealing of the graphene-metal stacks produced as a functional part of the devices.

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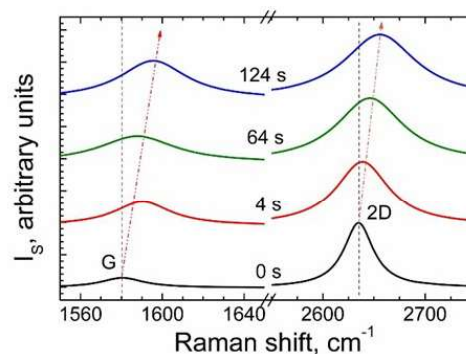


Fig. 1. Evolution of the Raman spectra with the annealing time (labels mean seconds) for the 1L graphene – Ni – film van der Waals contact.

Tuning of magnetoresistive properties of nanostructured manganite films

The magnetoresistive properties of nanostructured $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ films grown by pulsed injection metalorganic chemical vapour deposition technique on a special disordered glass-ceramics substrate were investigated. We fabricated and studied two series of films: (1) of thickness in a range of 25-900 nm deposited at a temperature of 750°C and (2) of thickness 400 nm grown at different deposition temperatures between 600°C and 775°C with a step of 25°C. The morphology and microstructure of the films were shown to depend on film thickness and deposition temperature. The thinnest film (25 nm) grows mainly in the amorphous phase, while thicker films have a well-pronounced structure of column-shaped crystallites with an average column width of 40-65 nm spread over entire thickness and separated by grain boundaries of 5-10 nm. The influence of growth conditions on the colossal magnetoresistance (MR) effect in these films was studied in pulsed magnetic fields up to 20 T. The dependence of MR on magnetic flux density was analysed using modified Mott's hopping model. We have shown that the films due to disordered grain boundaries behave as superparamagnetic material with reduced magnetic properties. The results shown in Fig. 2 demonstrate the possibility to tune the resistivity and MR of studied films.

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Hybrid tamm-surface plasmon polaritons mode for detection of mercury adsorption

Spectroscopic ellipsometry was used for the generation and study of the hybrid TPP-SPP mode as a sensor probe for the real-time formation of amalgam structures on the surface of a plasmon active gold layer. It has been shown that both the TPP and the SPP modes can coexist on the same metal layer if suitable conditions (metal layer thickness and angle of incidence) for both excitations are satisfied, and the coupling of these excitations results in the hybrid TPP-SPP mode. For TM polarised incoming light, both the TPP and the SPP are excited at different interfaces of the same metal layer, thus revealing the repulsive nature of these two resonances. The Au/Hg amalgam formation features and the penetration of the mercury atoms into the gold layer were determined using the experimental TIRE data and a regression analysis of a multi-layer model containing the index-profile amalgam layer. Green dots correspond to a real part of the conductivity of the Au/Hg layer at 700 nm wavelength (Fig. 3a). The hybrid TPP-SPP mode behaviour of the coupled excitations gave more information about the penetration of the mercury atoms into the gold layer than the single TPP and SPP resonances. The study demonstrates the possibility of applying the hybrid TPP-SPP mode for the design of advanced optical gas sensor technologies.

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Hot carrier approach to the Shockley-Queisser limit

The efficiency of a single-junction solar cell is limited by the Shockley-Queisser theory assuming that only photons with close to the band gap energy are used effectively, and the influence of hot carriers is taken into account only via thermalisation, i.e. lattice heating. Our experiment evidence the carriers to be heated by the intraband light absorption as well as by residual photon energy due to the electron-hole pair generation. The heating in the p-n junction gives rise to the hot carrier emf which has the polarity opposite to that of the classical generation-induced emf (Fig. 4, left) In this way, the competition of both photoresponse components may take place simultaneously (Fig. 4, right), and maximum reduction of the hot carrier emf leads to the increase of the efficiency of a p-n junction solar cell.

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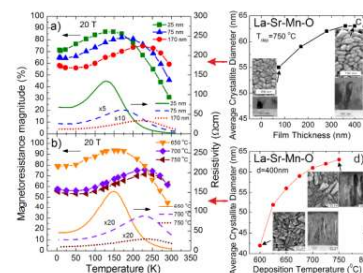


Fig. 2. Temperature dependences of magnetoresistance and resistivity (a, b) of $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ films with different morphology due to different thickness (c) and deposition temperature (d).

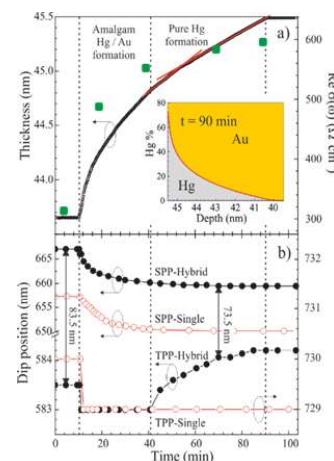


Fig. 3. (a) Thickness variation of the amalgam evaluated from a regression analysis of the hybrid TPP-SPP mode. The inset shows the depth profile of the gold and mercury at $t = 90$ min. (b) The experimental $\Psi(\lambda)$ dip position dependence on the exposure time of the gold surface in the saturated Hg vapour.

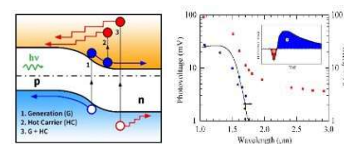
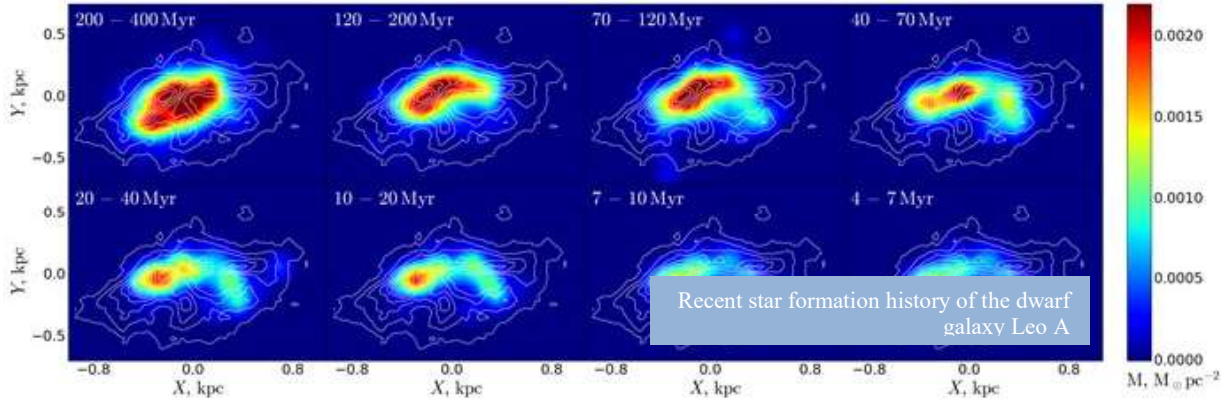


Fig. 4. (left) Rise of both emfs across the p-n junction. (right) Spectral dependence of both emfs across the GaAs p-n junction.



Star formation in dwarf galaxies restarts after billions of years of quiet

Dwarf galaxies are the building blocks from which larger galaxies are assembled. Therefore, understanding the processes shaping them is supremely important to the understanding of galaxy evolution as a whole. One of the mysteries of dwarf galaxies has long been the variety of their star formation histories: some galaxies formed most of their stars soon after the Big Bang, more than 10 billion years ago, while others have been forming them almost continuously throughout the age of the Universe, and still others have had two bursts of star formation, one early on and another several billion years later.

We have created a model that explains these, and many other, features of dwarf galaxy evolution. It turns out that the variety of properties is a result of the interplay between the growth of dwarf galaxy dark matter halos and the ionizing radiation field that permeates all space. The growth of dark matter halos is stochastic, meaning that even galaxies with the same halo mass at the present day may have experienced very different growth histories. Ionizing radiation exacerbates these differences: galaxies that collected most of their mass early were affected very little and could form stars throughout the age of the Universe; galaxies that were slow to grow their halos only formed some stars at very early times, before their gas was stripped away by radiation. Finally, galaxies that were small enough to be affected by radiation initially, but later grew large enough to be able to accrete gas again, can have two bursts of star formation – just like the galaxies Leo A and Aquarius (Fig. 1). Other properties of modelled galaxies, such as the relations between stellar mass and gas mass, metallicity and star formation rate, also agree rather well with observed dwarf galaxy properties (Fig. 2).

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Fig. 1. Star formation histories of real dwarf galaxies Leo A (top) and Aquarius (bottom) shown in red. Model galaxy star formation histories shown in black, with the dashed line showing actual model results and black histogram showing the same results binned in the same way as the observational data. The model galaxies were chosen to best match the observed ones – such objects are rare in the model, just as in the real Universe.

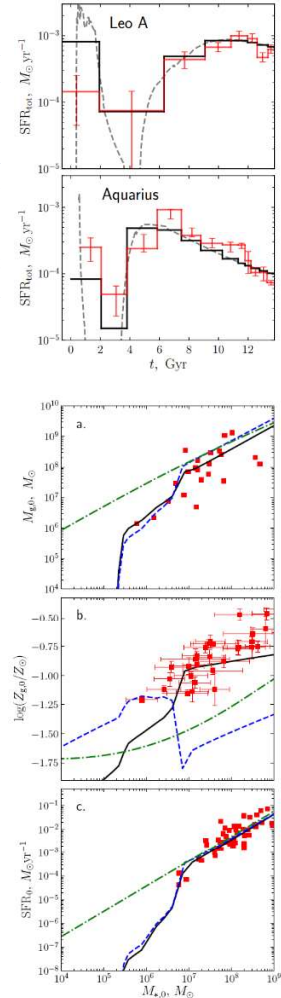


Fig. 2. Relations between parameters of real galaxies (points) and model galaxies (lines). From top to bottom, the relations connect stellar mass to gas mass, stellar mass to gas metallicity, and stellar mass to star formation rate. Black lines show our best-fit model; blue lines show a model where evolution of the metallicity of intergalactic gas is not taken into account; green lines show a model where the intergalactic ionizing radiation field is not taken into account.

Modeling

First-principles calculations of colour centers for quantum information processing

Electronic structure theory laboratory develops first-principles calculations for radiative and non-radiative transition in solids. A special emphasis is on point defects (also known as colour centers) for applications in quantum information processing, namely, quantum communication, quantum computing, and quantum-enhanced sensing. The examples of the defects we study are the nitrogen-vacancy center and the silicon-vacancy center in diamond or point defects in hexagonal boron nitride. One significant achievement of 2018 was the development of the first-principles methodology to calculate vibrational resonances associated with point defects in solids, in particular, their isotope shifts. We have proposed a correct procedure to extract these shifts from electronic structure calculations. The methodology was applied to the silicon-vacancy center in diamond (Fig. 1). This development will be advantageous in interpreting experimental luminescence and absorption spectra of various colour centers. In 2018 we also analysed most stable defects in hexagonal boron nitride. We have shown that frequently observed single-photon emission in these materials most likely originates from intra-defect transitions, and not band-to-defect transitions.

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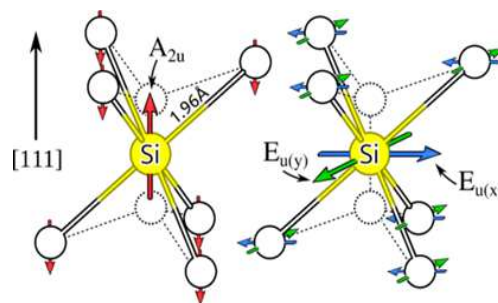


Fig. 1. A_{2u} and E_u – symmetry vibrations of the silicon-vacancy center in diamond.

Screening of point defects in methyllumonium lead halides: a Monte Carlo study

The organic sublattice of $\text{CH}_3\text{NH}_3\text{PbX}_3$ ($X = \text{I}, \text{Br}, \text{Cl}$) perovskites is believed to be related to the exceptional performance of the perovskite solar cells. We carried out modelling of the point defect screening by the CH_3NH_3^+ cations (dipoles) in this material. Our work is based on a statistical model with the (i) short-range, (ii) dipolar and (iii) long-range charge–dipole interactions between the defects and dipoles. The model is studied by the Monte Carlo simulations on a three-dimensional lattice. We investigate the charge screening in different structural phases of $\text{CH}_3\text{NH}_3\text{PbI}_3$ perovskite for various values of the charge-dipole interaction energy (e_{cd}). We demonstrate that a substantial interaction disturbs the antipolar long-range order of the CH_3NH_3^+ cations (Fig. 2) giving rise to a multidomain phase with a small electric polarisation.

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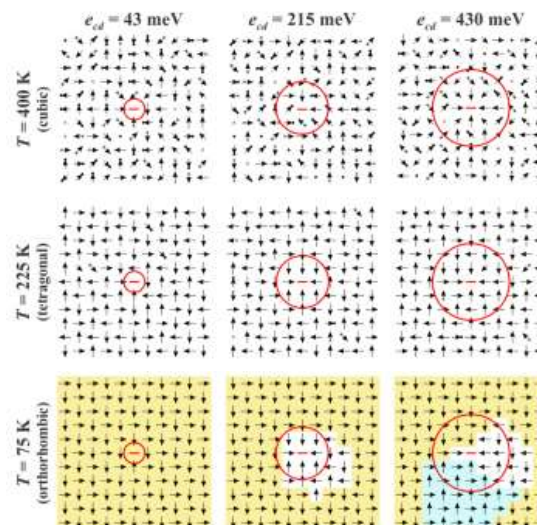


Fig. 2. The arrangement of dipoles around a single negative defect in the ab -plane at different temperatures and e_{cd} interaction energies. Temperatures correspond to the cubic, tetragonal and orthorhombic phases of $\text{CH}_3\text{NH}_3\text{PbI}_3$. The domains of dipoles at 75 K are shaded in different colours. The red circles around the defects mark the apparent screening radius.



Nonlinear dynamics and chaos

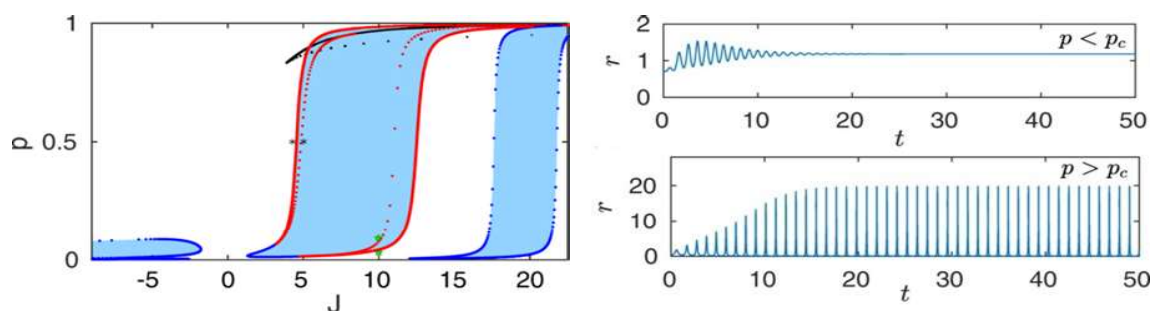


Fig. 1. Aging transition in a network of quadratic integrate-and-fire (QIF) neurons with distributed-delay synaptic coupling. (Left) The bifurcation diagram in the (J, p) plane derived from a macroscopic network model. Here J denotes the strength of synaptic coupling and p is the proportion of inactive (quenched) neurons in the population. The black dots represent the saddle-node bifurcation. The red and blue dots show the supercritical and subcritical Andronov-Hopf bifurcations, respectively. The red solid curve indicates the limit point of cycles bifurcation. The colored regions correspond to macroscopic oscillations of the firing rate and the mean membrane potential. (Right) The dynamics of the spiking rate. In certain regions of the parameters, a counterintuitive effect of aging induced oscillations is observed, when an increase in the proportion of nonspiking neurons induces macroscopic oscillations. The oscillations do not appear if the proportion of inactive neurons is too small, $p < p_c$ (top), while for $p > p_c$, the network starts to generate oscillations (bottom).

Macroscopic oscillations of a QIF neuron network with global distributed-delay coupling

Studies of collective behaviour in systems consisting of many coupled nonlinear dynamic units is an active area of research in diverse fields ranging from physics to neuroscience. We considered a large network of globally coupled QIF neurons, which are canonical representatives for a class I neurons near the spiking threshold. The model includes two heterogeneous parameters. One of them characterises the state of isolated neurons and subdivides them into spiking and excitable (nonspiking) units. The other heterogeneous parameter is the interaction delay time. The introduction of heterogeneous interaction delays is motivated by the fact that in realistic neural networks axons have different lengths and are characterised by different transmission speeds, which leads to different signal transmission times between neurons. In the thermodynamic limit (an infinite number of neurons), we reduced the model to a simple system of ordinary differential equations for the macroscopic order parameters. By bifurcation analysis of these equations, we identified the regions in the parameter space where the network exhibits macroscopic self-oscillations. We also analysed the influence of interaction delays on the ageing transition. The ageing transition characterises the robustness of the macroscopic self-oscillations against damage that increases the proportion p of inactive neurons in the network. When this proportion is increased to some critical value p_c , the network loses its oscillatory dynamics. We showed that the interaction delays considerably complicate the phenomenon of the ageing transition. Because of the delays, the ageing transition has a resonance-like structure in the dependence of the coupling strength. More importantly, we revealed a striking feature that contradicts with the conventional definition of the ageing transition. In some parameter regions, we found out that the presence of nonspiking neurons is necessary to gain macroscopic oscillations, i.e., the oscillations appear only when the proportion p of inactive neurons exceeds some critical nonzero value p_c , while for $p < p_c$ there are no oscillations (Fig. 1). Such ageing-induced oscillations are counterintuitive and, to our best knowledge, they have not been observed in previous studies of the ageing transition. We compared the solutions of the macroscopic equations with the numerical simulations of the microscopic model. For a network consisting of 5000 QIF neurons, we got an excellent agreement between the above two solutions. In addition, by numerical analysis of the macroscopic equations in different parameter regions, we found the collective chaos regime (Fig. 2) and confirmed its existence by direct numerical simulation of the microscopic model.

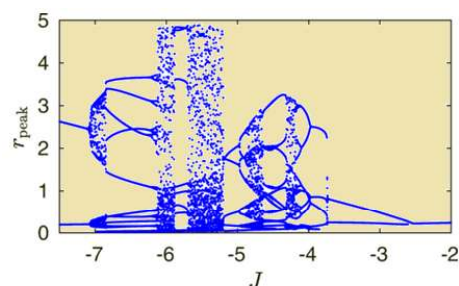


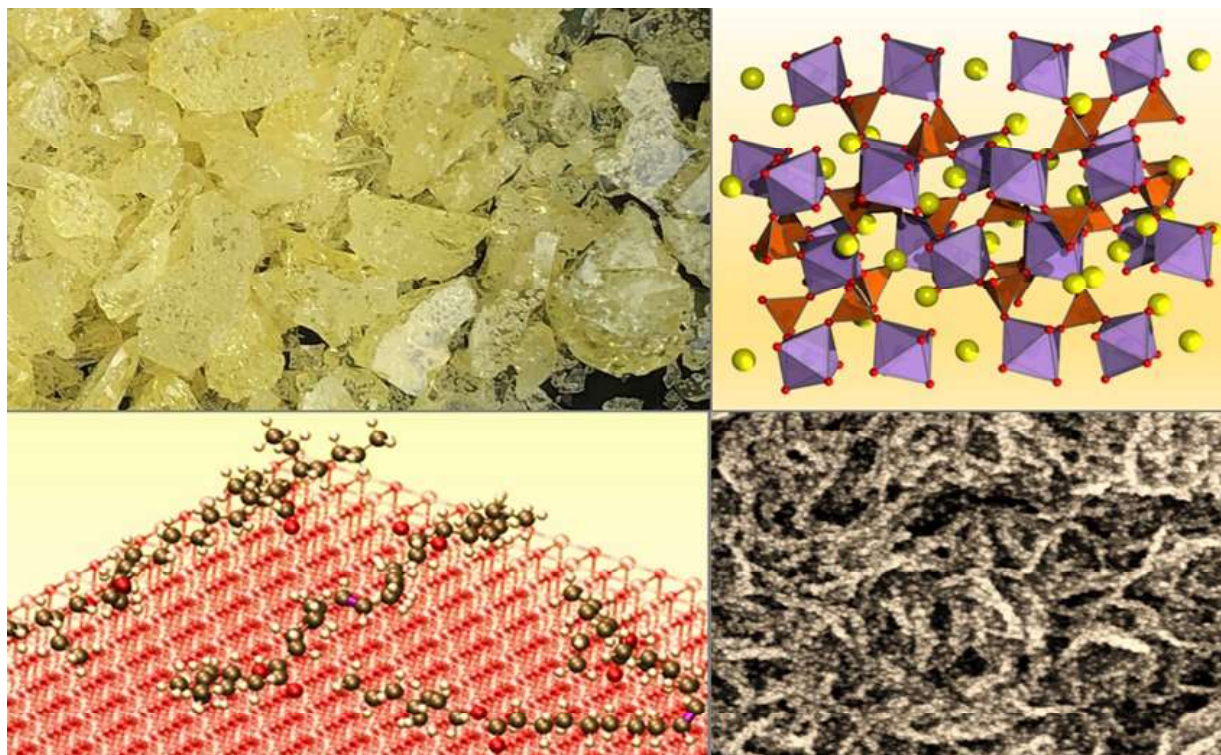
Fig. 2. One-parameter bifurcation diagram derived from the macroscopic model. The peak values of the spiking rate are shown as functions of a smoothly varying coupling strength J . The areas, in which the peak values are scattered, correspond to the regime of collective chaos.

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Electrochemistry & tribology



Electrochemical materials science

The R&D activities in this area are focused on the application of electrochemical methods for the development and characterisation of new functional materials such as:

- alloys of light and refractory metals (Mg, Al and Cr, Nb, Zr, Ta) with controllable corrosion resistance;
- semiconductor nanowires loaded in the alumina pores and nanostructured titanium or iron oxides
- transparent conductive oxide layers and their heterostructures;
- superparamagnetic and luminescent nanoparticles with possible applications in nanomedicine;
- new efficient materials for photovoltaic, nanoelectronic and energy storage technologies;
- smart coatings with active corrosion protection ability for metals in aggressive environments.

Electrochemical, chemical as well as physical (magnetron sputtering, atomic layer deposition) methods are applied for the surface modification and production of smart materials with exceptional anticorrosive, electrocatalytic, magnetic, mechanical or other properties. The integral part of the process of new materials development is a thorough characterisation of their structure, morphology and chemical composition. Environmental friendliness is imperative for all newly developed technologies.

Another trend of scientific research is related to tribology and formation of compositions of biofuels, lubricants and plasticisers, using biodegradable components. These activities include a search for tribologically efficient materials for new type anodic aluminium coatings with exceptional resistance to friction and attrition. The results are tested directly in the 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 in metals, alloys, composite coatings, paints and lacquers in the natural and artificial atmosphere as well as testing of microbially induced corrosion of materials in atmosphere and model medium.



Electrochemical synthesis of photoactive carbon-carbide structure on silicon in molten salt

Carbon-carbide structures are promising for increasing the light-harvesting performance of Si-based solar cells. The structures on porous Si showed low reflectance, increased hardness and improved photo-efficiency. Chemical or physical vapour depositions, as well as various etchings, are typically used to improve the antireflection performance of Si-based solar cells. These techniques, however, are not cost effective and include hazardous and expensive reactants. We synthesised electrochemically C-SiC coatings on silicon with a distinctively developed surface in molten CaCl_2 at 850 °C. Mott-Schottky analysis showed p-type semiconductivity of the structure with a high density of charge carriers $N > 10^{16} \text{ cm}^{-3}$. The surfaces absorbed over 90% of white light and showed high photo-activity. The composite is promising as an antireflection and protective coating or photo-electrode. Part of the results was obtained in collaboration with the researchers at Cambridge University (UK). The research leading to these results has received funding from the EC Seventh Framework Programme under grant agreement PIOF-GA-300501.

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Rapid screening method to evaluate lubricant durability

Typically, it is overly costly to assess the durability of lubricants in heavy duty equipment because of energy, labour, depreciation and other expenses. A simple method, which uses thin oil film degradation on metal surfaces, was developed at Tribology Laboratory to compare oil stability. The films with thicknesses from 20 to 500 μm were tested to investigate the effects of oxidation, hydrolysis, saponification and other degradation processes. Spectroscopy, chromatography and microscopy were used to further study of the degradation kinetics. In addition, many brand-name lubricants were compared side-by-side per requests from the gas generator, transmission, hydraulic fluid and engine oil users (Fig. 2). Europe's leading lubricant magazine "Lube" invited FTMC to describe this method in their centrefold article published in June 2018.

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Computational investigation of lithium intercalation into $\text{Li}_{1+x}\text{Ti}_2\text{O}_4$ spinel structures

Metallic $\text{Li}_{1+x}\text{Ti}_2\text{O}_4$ spinels are studied using the density functional theory as model systems for the complex environments of electrode/electrolyte interfaces in lithium-ion batteries. The calculated activation energies for the formation of $\text{Li}_2\text{Ti}_2\text{O}_4$ at the surface are found to be much lower than for Li diffusion through bulk LiTi_2O_4 , suggesting a two-phase lithiation process taking place during battery operation. Additionally, the delithiation reaction mechanism in $\text{Li}_2\text{Ti}_2\text{O}_4$ is studied by evaluating the free energies for Li^+ transfer to an ethylene carbonate electrolyte by employing a Born-Haber thermodynamic cycle. The effects of an applied (external) potential are incorporated into the thermodynamic cycle and provide means to calibrate the electrode bias potential to the experimentally known scale. Finally, the effects of an applied electrode potential are studied on the $\text{Li}_2\text{Ti}_2\text{O}_4$ delithiation energetic pathways in various environments emphasising the different contributions to the charge transfer energetics in such electrode materials.

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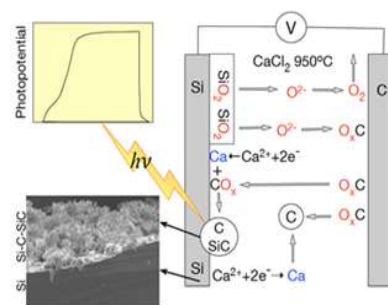


Fig. 1. Schematic diagram of the electrochemical synthesis of Si-C-SiC surface structure.

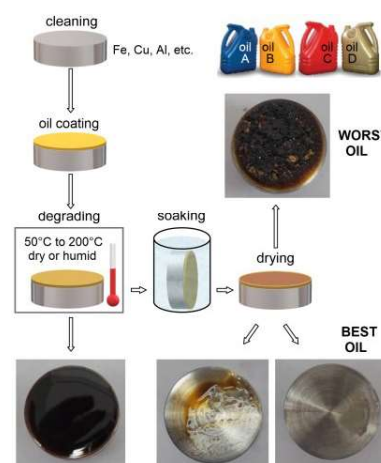


Fig. 2. Simplified scheme of the thin film test, developed at FTMC Tribology laboratory, to compare degradation trends of various oils.

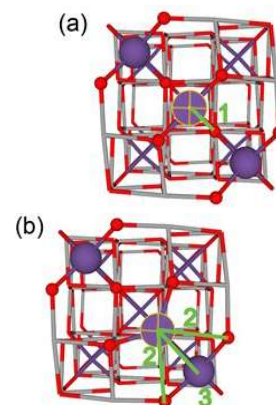
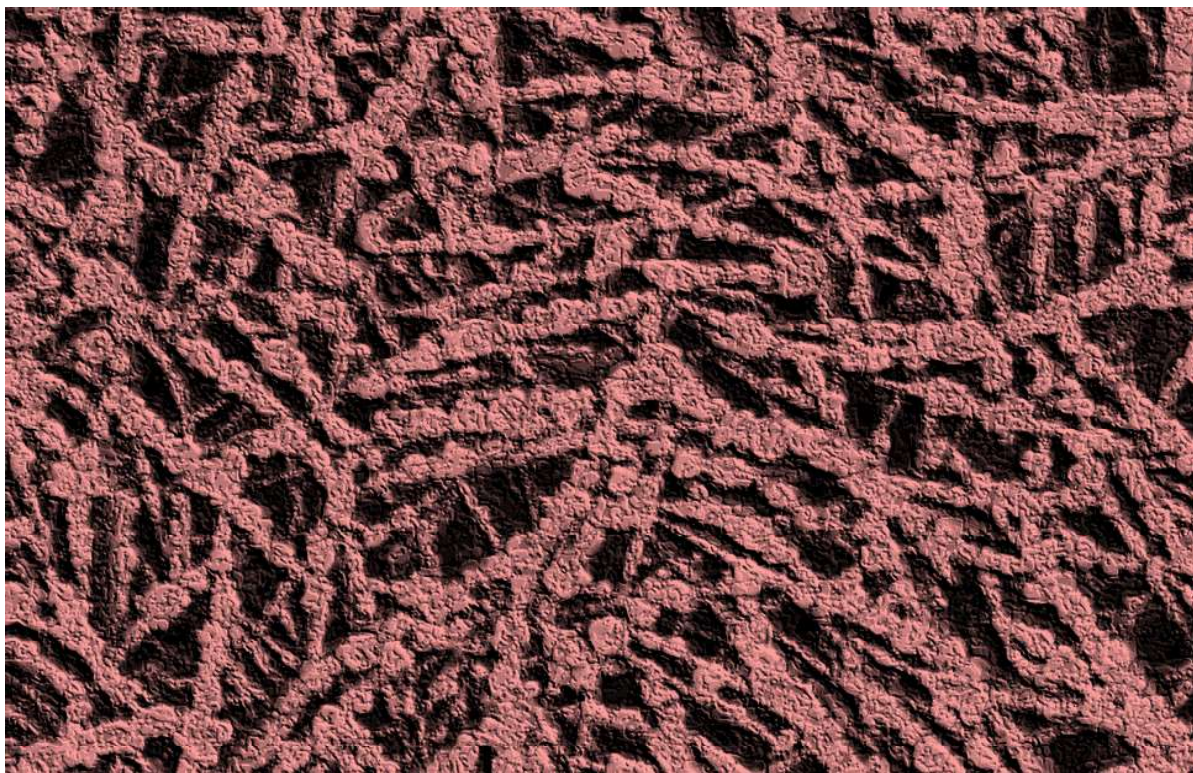


Fig. 3. Top view of stable surface structures at symmetrically terminated (100) face of LiTi_2O_4 .

Materials for catalysis



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

Electroless metal plating is a well-known method for deposition of metal coatings by a controlled chemical reduction and formation of small (nano-scale) metal particles. The autocatalytic metal ion reduction systems are widely used for decorative and functional purposes, i. e. for deposition of a conductive metal layer on dielectrics, semiconductors or conductors with a complicated configuration without external current. The selection of suitable reducing agent and conditions of the reaction (temperature, the concentration of the reacting substances, etc.) plays a crucial role for creating of stable solutions and obtaining coatings with required characteristics, such as purity and surface roughness. The use of conventional hydrogen-containing reducing agents is connected with environmental and technological problems: (i) the plating bath cannot be recycled, i.e. the reducing agent oxidises irreversibly; (ii) the plating rate and solution stability are not high enough. For these reasons, the search and investigations of the reducing agents of a new type, e. g. charge-transfer reducers, namely the different oxidation state metal-ion redox couples, are actual nowadays, and they are developed and applied in the Department of Catalysis. The main reducing agents used are Ti(III) and Co(II), which oxidise during the electroless plating processes to Ti(IV) and Co(III). An additional advantage of such systems, where no hydrogen is formed during the electroless plating process, is the possibility to reduce the oxidised form of the reducing agent to the initial state. The R&D activities of our department in this area are focused on the development of new electroless metal plating processes as well as fundamental studies of reactions occurring in autocatalytic metal ions reduction systems using electrochemical quartz crystal microgravimetry. The electroless metal plating method is also successively used for fabrication of new catalytic materials for fuel cells. The non-noble metal and noble metal catalysts with a low amount of noble metal-supported titanium, titania nanotube arrayed surfaces, carbon, graphene powder or other supports with enhanced activity towards the oxidation of various fuels, have been developed. The catalysts obtained are promising anode materials and can be used in the practical fuel cells.

Development of sodium borohydride and hydrazine fuel cells

The interest in low-temperature fuel cells (FCs), including direct sodium borohydride (NaBH_4) fuel cells (DBFCs), as well as direct hydrazine (N_2H_4) fuel cells (DHFCs), has been growing over the past decades. A low-cost and straightforward approach was used for fabricating of an efficient anode catalyst for DBFCs and DHFCs. We employed fiber-shaped cobalt (Co_{fiber}) coating deposited on the copper surface as the support for the deposition of Au nanoparticles. It has been determined that the deposition of low amounts of Au nanoparticles on the fiber-shaped Co coating resulted in an enhanced peak power densities for the direct $\text{N}_2\text{H}_4\text{-H}_2\text{O}_2$ and $\text{NaBH}_4\text{-H}_2\text{O}_2$ fuel cells as compared to those of pure $\text{Co}_{\text{fiber}}/\text{Cu}$. Peak power densities up to 162 mW cm^{-2} for $\text{N}_2\text{H}_4\text{-H}_2\text{O}_2$ and 188 mW cm^{-2} for $\text{NaBH}_4\text{-H}_2\text{O}_2$ were obtained at a temperature of 25°C using the $\text{AuCo}_{\text{fiber}}/\text{Cu}$ anode catalyst with the Au loading of $84.4 \mu\text{g}_{\text{Au}}\text{cm}^{-2}$.

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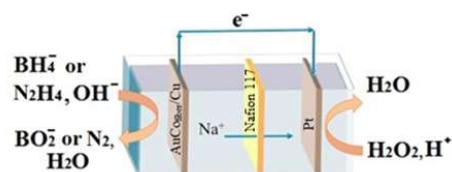


Fig. 1. Schematics of the assembled direct $\text{NaBH}_4\text{-H}_2\text{O}_2$ or $\text{N}_2\text{H}_4\text{-H}_2\text{O}_2$ fuel cells.

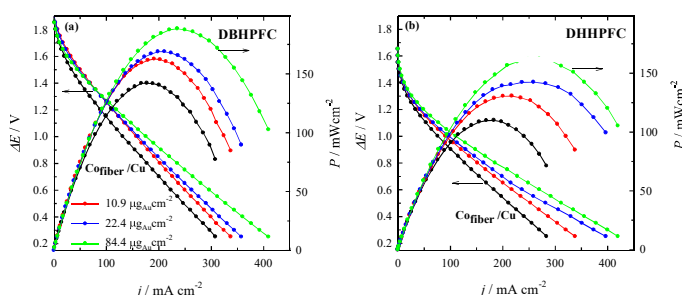


Fig. 2. Cell polarization and power density curves for DBHPFC (a) and DHHPFC (b) using the $\text{Co}_{\text{fiber}}/\text{Cu}$ and different $\text{AuCo}_{\text{fiber}}/\text{Cu}$ anode catalysts with the anolyte consisting of 1 M NaBH_4 (a) or 1 M N_2H_4 (b) in 4 M NaOH and 5 M H_2O_2 + 1.5 M HCl catholyte at 25°C .

Development of catalysts for hydrogen generation

On a global scale, hydrogen energy is considered as an almost perfect strategy for mitigating energy and environmental challenges. Hydrogen is a clean and environmentally friendly energy source for the future, with wide-ranging applicability in heating, transportation, mechanical power, and electricity generation. Herein, we use a simple method for the fabrication of an efficient Co-based catalyst for the hydrolysis of sodium borohydride. A fiber-shaped Co coating was electroplated on a treated Cu surface, followed by deposition of Au or Pt crystallites on the Co coating by the galvanic displacement technique. The deposition of Au or Pt crystallites on the Co coating resulted in significantly enhanced catalytic activity for the hydrolysis of NaBH_4 in alkaline conditions, as compared to that of a bare fiber-shaped Co coating. Moreover, the highest hydrogen generation rates of $1238.3 \text{ L min}^{-1} \text{ g}_{\text{Pt}}^{-1}$ and $1012.3 \text{ L min}^{-1} \text{ g}_{\text{Au}}^{-1}$ were obtained for the $\text{PtCo}_{\text{fiber}}/\text{Cu}$ and $\text{AuCo}_{\text{fiber}}/\text{Cu}$ catalysts (corresponding to Pt and Au loadings of $28.7 \mu\text{g cm}^{-2}$ and $20.0 \mu\text{g cm}^{-2}$), respectively, at a temperature of 70°C .

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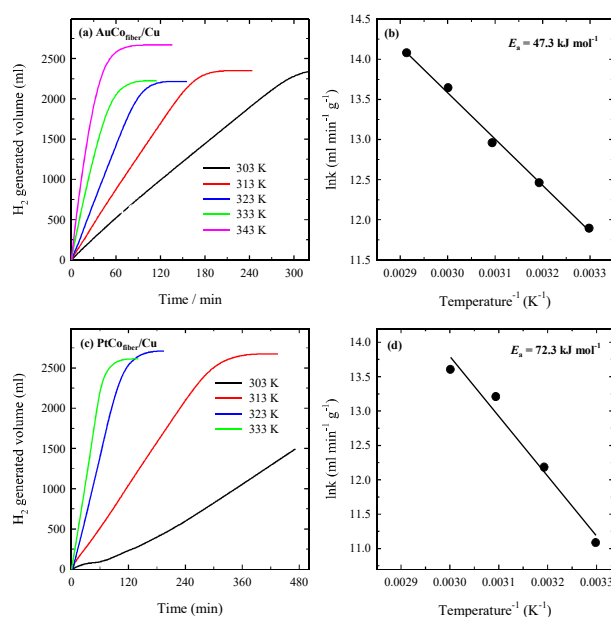
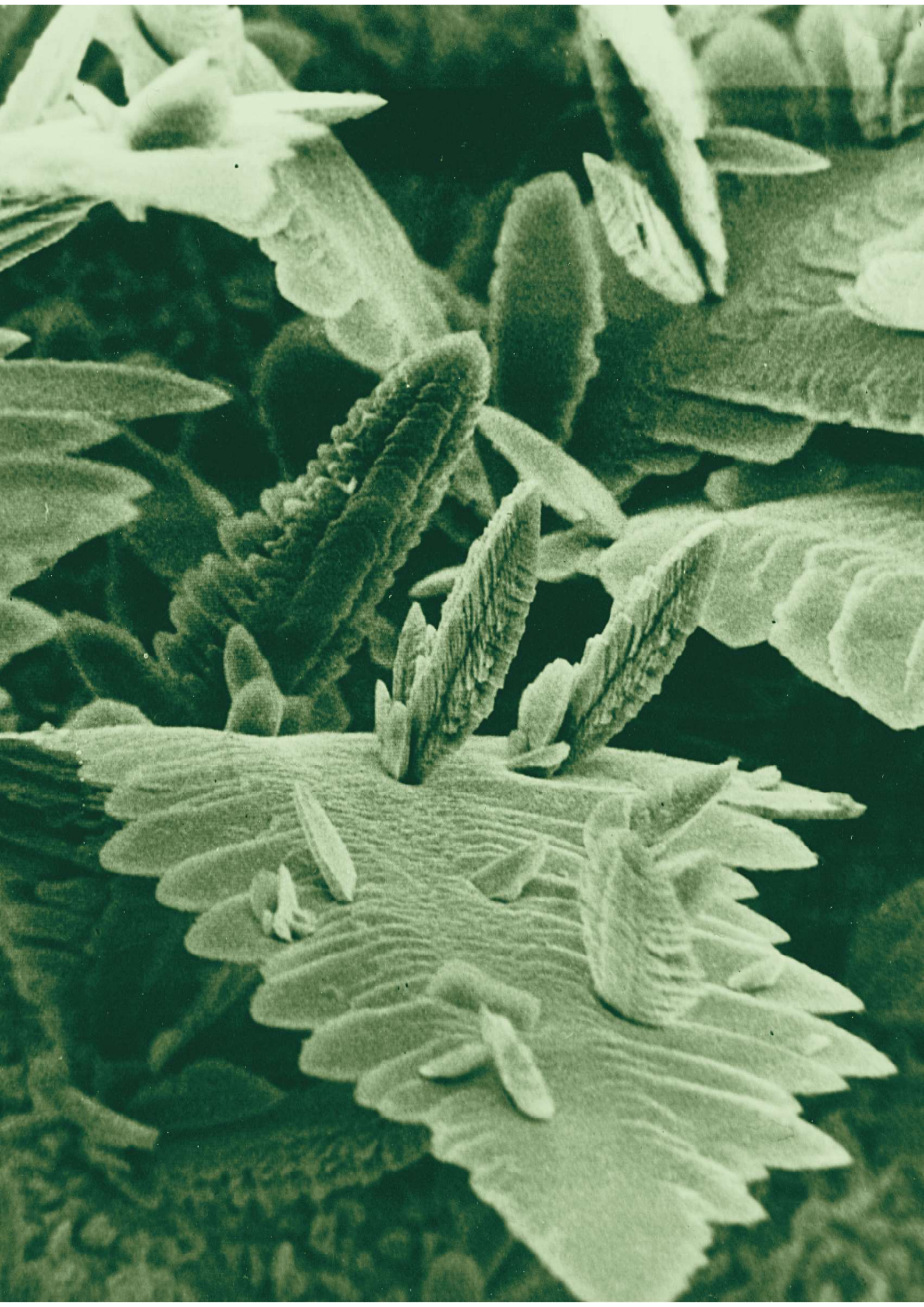
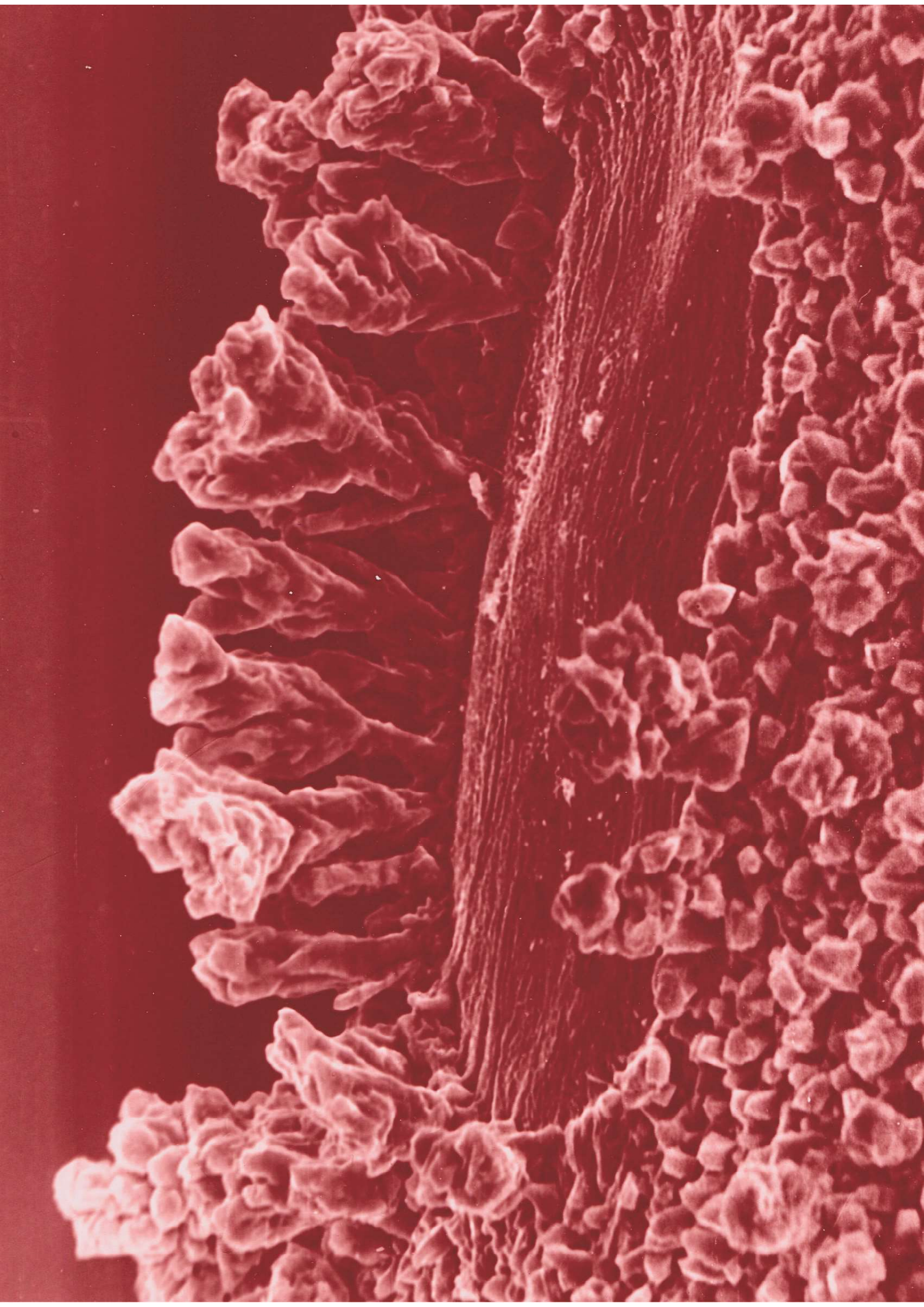


Fig. 3. H_2 generation from 15 ml 5 wt.% NaBH_4 + 0.4 wt.% NaOH catalysed by the $\text{AuCo}_{\text{fiber}}/\text{Cu}$ with the Au loading of $28.0 \mu\text{g}_{\text{Au}} \text{cm}^{-2}$ (a) and the $\text{PtCo}_{\text{fiber}}/\text{Cu}$ with the Pt loading of $28.7 \mu\text{g}_{\text{Pt}} \text{cm}^{-2}$ (c) at different temperatures. (b, d) The Arrhenius plots calculated from the rates of NaBH_4 hydrolysis in the same solution.





Environment



The environmentally-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 environmental physics and chemistry, environment contamination and climate changes.

Tasks:

- 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 and characterization of the impact of environment contamination on climate change.
- 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.

Scattering properties of atmospheric aerosol particles from 28 ACTRIS sites

The Preila environmental pollution research station (PLA) is one of the ACTRIS stations. The data in Fig. 1 (b-e) include particle light scattering (σ_{sp}) and hemispheric backscattering (σ_{bsp}) coefficients, scattering Ångström exponent (SAE), backscatter fraction (BF) and asymmetry parameter (g). The PLA registered σ_{sp} values (medians > 40 Mm⁻¹) are higher compared to both other Nordic and Baltic stations and other coastal sites (e.g. Mace Head (MHD) and Finokalia (FKL)) which are among the highest in Europe. High g values are also observed in PLA, BIR, JFJ and DEM stations which demonstrate an average of fine aerosol particles (with SAE values similar to or higher than 1.5).

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Global analysis of continental boundary layer new particle formation

Atmospheric new particle formation (NPF) is an essential phenomenon of global particle number concentrations. Thus, the frequency of NPF, formation rates of 10 nm particles (J_{nuc}), and growth rates (GR) in size range of 10–25 nm using at least one year of aerosol number size-distribution observations at 36 different locations around the world were studied. The annual and seasonal frequency of the NPF formation events at the various measurement sites are presented in Fig. 2, where the dashed lines in panels (Fig. 2(b-e)) show the median seasonal values, and the colour scheme represents the classification of the sites into polar, high-altitude, remote, rural, and urban environments. It has been found that the connection among J_{nuc} , GR, and NPF event frequency was at best moderate among the different measurement sites, as well as among the sites belonging to a particular environmental regime.

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Tree-ring formation as an indicator of forest capacity to adapt to the main threats of environmental changes in Lithuania

Air pollution and climate change effects on a forest's capacity to adapt to and mitigate the main threats from global changes constitute significant current scientific research foci. The pollutant load from 2000 significantly decreased as a result of the decrease in emissions in Europe, including Lithuania, except for NO₃ air concentrations and deposition (Fig. 3). O₃ concentration has also had a tendency to decrease since 1996 and has made about 0.3 µg m⁻³ per year and >0.4 µg m⁻³ per vegetative stage (V-VIII). Between 2005 and 2015, the level of NH₄ deposition increased up to 250 mgNm⁻² and was mainly attributed to an increase in the activity in Lithuanian rural development.

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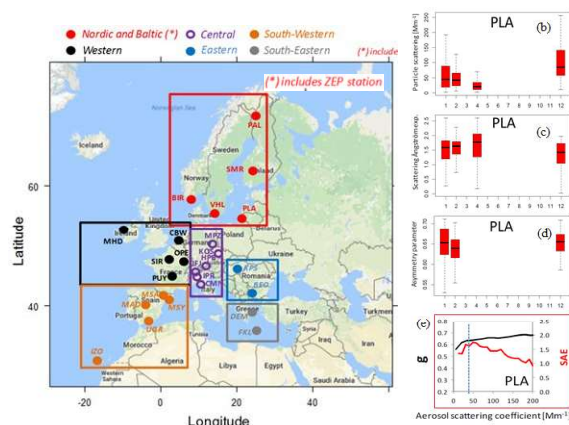


Fig. 1. (a) Locations of ACTRIS stations. Seasonal cycles of (b) σ_{sp} , (c) SAE, and (d) g. (e) Scatter plot between σ_{sp} (x axis) and SAE (y axis; red) and g (y axis; black).

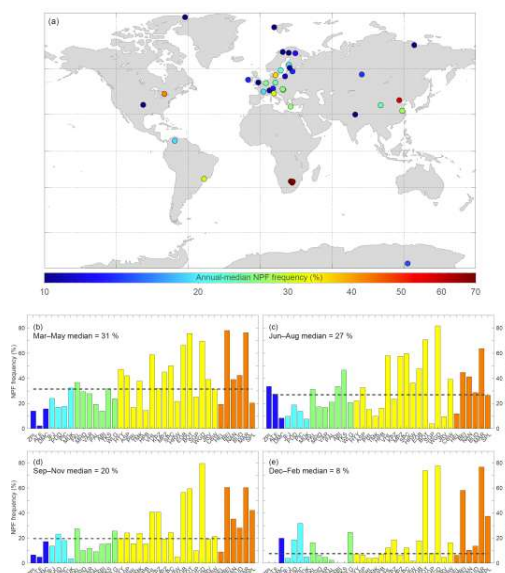


Fig. 2. Annual-median (a) and seasonal-median (b-e) frequency of the NPF formation events in different measurement sites.

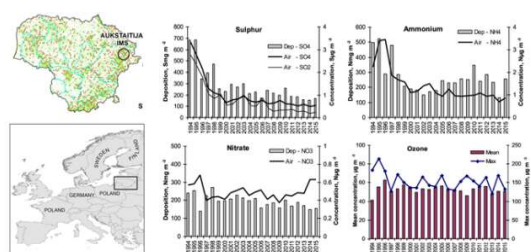
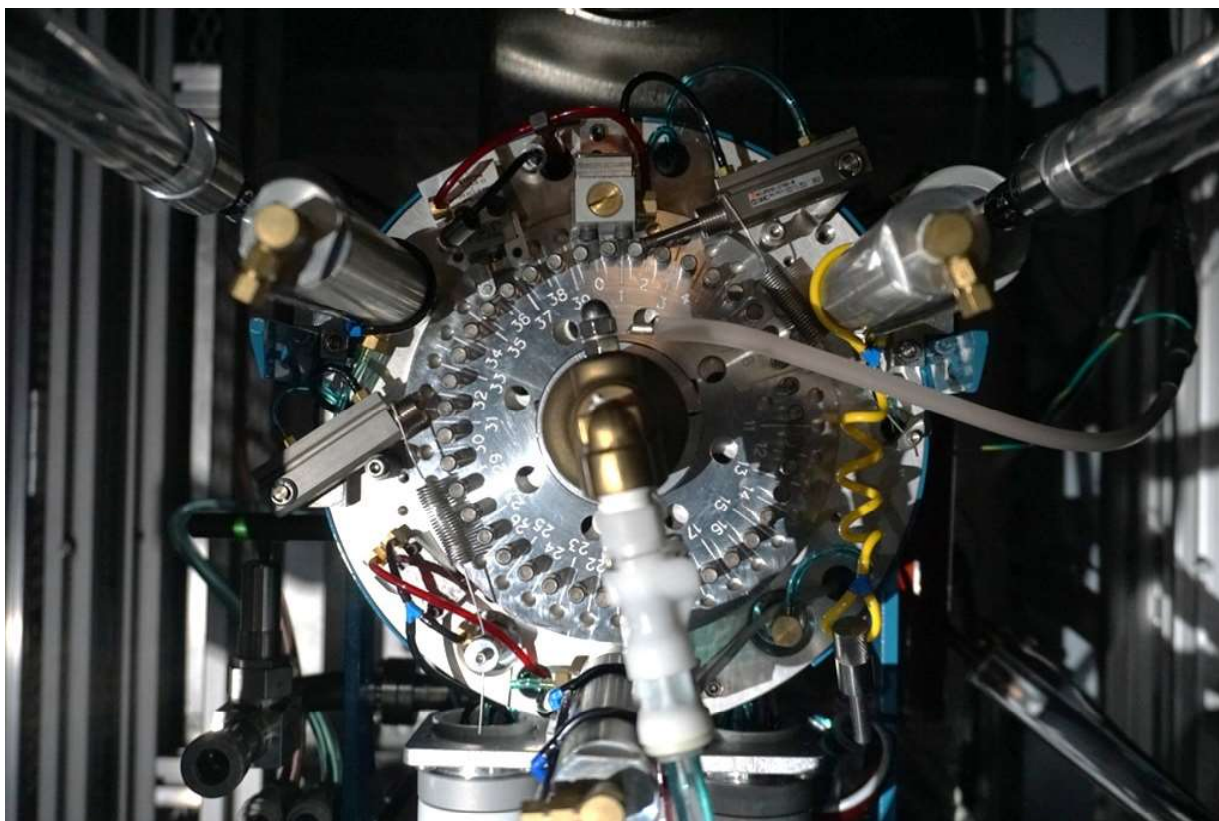


Fig. 3. Location of National Forest Inventory plots in Lithuania (Aukštaitija IMS) and changes in the main air pollutant concentrations and acid depositions from 1994 to 2015.



Nuclear research for actual applications today and innovative technologies for future

The Department of Nuclear Research develops and applies known and innovative technologies and methods in the fields of experimental nuclear spectroscopy, nuclear energy safety, radiation protection, radiochemistry, mass spectroscopy, Mössbauer spectroscopy, ion beam analysis and material modification. The keystones of the safety field are the safe operation assurance of nuclear facilities, the optimisation of radioactive waste management, the assessment of shielding materials and comprehension of processes of radionuclides transport through engineering barriers to enable nuclear facility safety. The special attention is paid to environmental impact assessment of energy generating facilities, elemental and isotopic analysis of groundwater, food fabrics and products and also industrial stocks, medical samples with sensitivity up to 1 ppq (for non-interfered isotopes). Application of stable isotope ratio analysis ($\delta^{13}\text{C}$, $\delta^{15}\text{N}$, $\delta^{18}\text{O}$ and $\delta^{34}\text{S}$) in environmental, biomedical and food samples stimulates new promising technologies. The ^{14}C measurements open the potentially new field of activity related to carbon dating and analysis of triple carbon ratio for dedicated samples. Complementary 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 an essential part of our activities having intersection both with semiconductor materials and applications for lasers. Investigation of organic scintillator films opens new possibilities of simple scintillator material application for detection and spectroscopy of ionising radiation particles. In search of future practical applications, the high energy electromagnetic radiation generation is investigated using ultrashort laser pulses.

Advanced technologies for radioactive waste characterisation

Optimisation of nuclear facility radioactive waste (RW) management by applying grouping and separation of RW using modelling and experimental analysis of RW nuclide content from nuclear power plants (NPP) is one of the keystones ensuring smooth and successful NPP decommissioning process. The concentration of activation products in the reactor construction materials (graphite, fuel channels, internal reactor constructions, CPS rods, biological shielding materials) strongly depends on the conditions of the activation. The MCNP6/SCALE6.2 modelling, providing neutron flux distribution in the 3D RBMK-1500 reactor and activation of materials, and the results of experimental measurements, allowed us to separate waste streams into highly activated zones (red line), zone of intermediate and low activation metal construction, biological shielding materials, and non-activated materials for which only surface contamination is relevant (Fig. 1). The nuclide vectors to obtain the nuclide composition in every radioactive waste stream have been determined. The scaling factors (Fig. 2) are based on the empirical dependence between specific activities of nuclides in the investigated samples of analysed waste streams.

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Express method of specific ^{14}C activity determination

The novel express-analysis method for specific ^{14}C activity determination in small graphite samples of 1-100 μg range can be used for radiological characterisation of radioactive waste or biomedical applications. The method applies an oxidation procedure to remove the ^{14}C (CO_2) from the different carbonaceous matrixes in a controlled manner. The method was verified using a liquid scintillation counting (LSC) technique. Specific ^{14}C activity determination procedure takes ~ 10 min. The method can be applied for ^{14}C characterisation in irradiated graphite during the dismantling of graphitic constructions and sorting of radioactive graphite waste from decommissioned nuclear power plants.

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Identification of air pollution sources using mass spectrometry methods

Research of aerosol particles, collected during winter sampling campaigns at a coastal site (Preila), has revealed a dependence of the particles origin on the air mass direction. The received organic mass spectra provide strong evidence that shipping emissions are a significant source of organic matter at this coastal site during dominant marine air mass. Meanwhile, during dominant continental air masses, we were able to identify fossil fuel burning, as a predominant source of the less refractory organic matter in the smallest particles, and biomass burning as predominant source of a more refractory organic matter in the larger size particles.

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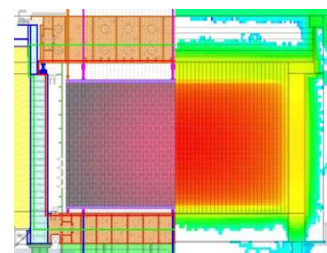


Fig. 1. Separation of activation zones according to neutron flux in RBMK-1500 reactor.

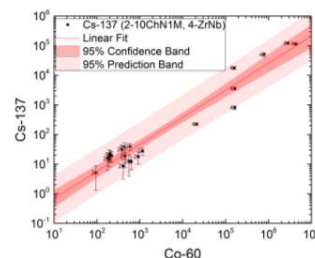


Fig. 2. Experimental data analysis for the determination of scaling factors in the radioactive waste of RBMK-1500 metal components.

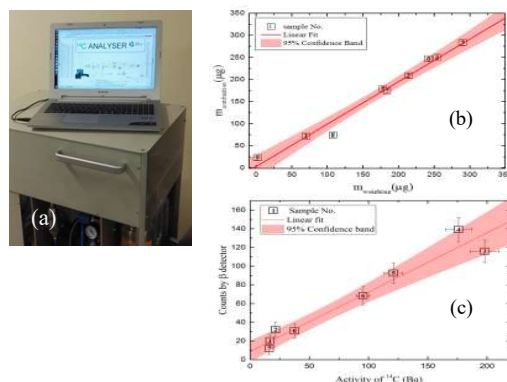


Fig. 3. (a) Analyser for the specific ^{14}C activity determination. (b) Sample mass determined by two independent methods. (c) Correlation between LSC and semiconductor detectors.

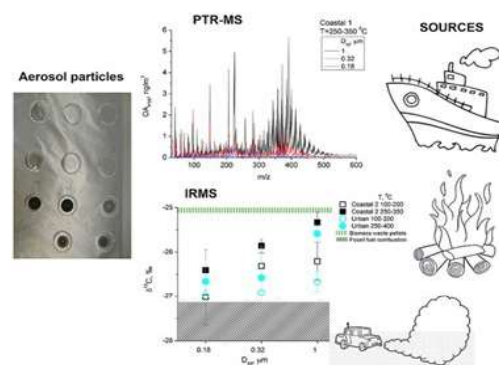


Fig. 4. Air pollution sources identified by mass spectrometry methods.

Advanced technologies for tracing of ^{14}C concentration variations in the environmental samples

Applications related to radiocarbon, such as single state accelerator mass spectrometry, allows us to observe small changes of ^{14}C in environmental samples. It is an excellent tool for assessing the rate of eutrophication processes in water ecosystems identifying potential systemic errors in radiocarbon dating. Radiocarbon ^{14}C and $\delta^{13}\text{C}$ were measured in the Tapeliai lake sediments core to trace the rate of eutrophication processes. Two fractions of humin and humic acid were used in this study. It was assumed that radiocarbon dating of bottom sediments does not give us a reliable radiocarbon age as there are too many processes that influence the origin and cycling pathways of organic and inorganic carbon. However, the data of ^{14}C obtained from sediments have revealed the influence of the hydrological changes in the lake system. According to the ^{14}C records of the sediments core, it is clear that at the beginning of the XX century, a huge impact of old dissolved organic carbon was delivered to the lake. As a result, the “reservoir effect” had changed drastically – it dropped from 1330 BP to 2360 BP and lasted for 50 years. Another breaking point in the ^{14}C records was observed in 26 cm depth. According to the sedimentation rate (estimated from ^{210}Pb), this depth corresponds to the date of 1950 (^{14}C from 75 pMC to 87 pMC). Major events: a) ^{137}Cs profile indicated nuclear weapon test; b) blocked ditch resulted in no old DOC delivered to the lake basin. The ^{14}C content in the lake sediments reached previous value (85 pMC in 1900-ies) in recent 30 years and shows a stable trend with minor changes.

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Regional aerosol source apportionment using stable carbon and radiocarbon analysis

The combination of the stable carbon isotope ratio ($^{13}\text{C}/^{12}\text{C}$) with radiocarbon data (^{14}C) allowed us to distinguish coal, liquid fossil fuel combustion, and non-fossil derived aerosol particle emissions. Isotope mass balance calculations revealed that the traffic emissions comprised 15% and 25% in rural and urban sites, respectively, and did not depend on a season. The input from coal-derived aerosol particles was estimated to be 15% at an urban site during the cold period.

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Isotope ratio mass spectrometry to trace biogenic pollution

Each chemical reaction has its own fractionation factor – any variations in isotope composition in living organisms display the respond of the metabolic processes of the organism to environmental change. Cormorants transport nutrients from water to the land ecosystem and pollute biogenically. Research of $\delta^{13}\text{C}$ and $\delta^{15}\text{N}$ data of small mammal hair in three cormorant colonies showed the amount of influence of bird colonies to all ecosystem and suggested control strategies.

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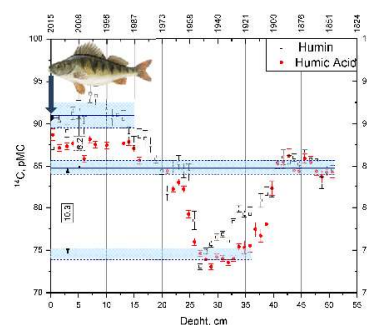


Fig. 5. Tracing of ^{14}C variation in the lake sediments caused by environmental factors. The reservoir age for the Tapeliai lake system was estimated to be 927 ± 45 years using the first-year perch as a sample (caught in March of 2018).

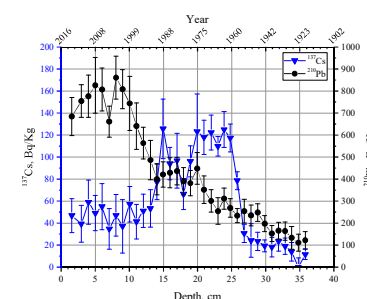


Fig. 6. The ^{137}Cs and ^{210}Pb measurements in the sediments.

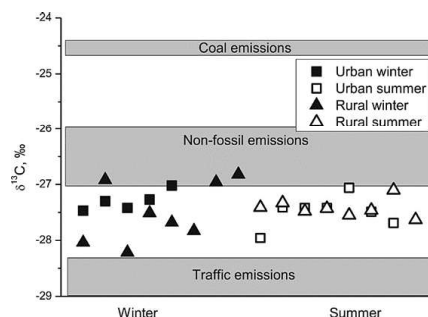


Fig. 7. The $\delta^{13}\text{C}$ values in a total aerosol PM1 fraction, collected in urban (Vilnius city) and rural (Vaiksteniai) locations during winter (2015) and summer (2016) seasons.

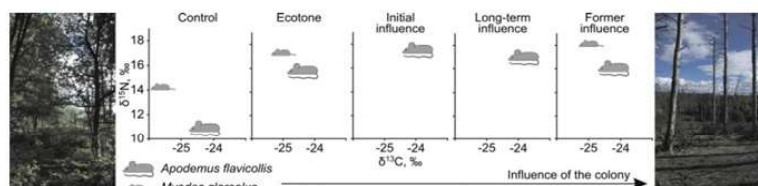


Fig. 8. The impact of Great Cormorants on biogenic pollution of land ecosystems: stable isotope signatures in small mammals.



Textile technologies



Advanced textile materials

Developing of new advanced materials and smart textile products based on combining different technologies such as robotics, bio- and nano-technologies, information technology, mechatronics and others is a core of investigation in the Textile Institute. 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 textile garments friendlier for the surrounding environment. The investigation is focused on textile materials with functional and multifunctional properties processed by plasmochemical surface treatment, coating technologies and micro and nano-finishing, smart textile garments with active thermoregulation using bio-ceramics, PCM and wearable electronics and numerical modelling. These investigations make the background for the development of protective clothing technologies where the heat exchange in textile garments, ballistic impact, electroconductive and EMR shielding materials take a significant role in their performance.

Participation in the ACAMSII project, initiated by European Defence Agency, encouraged investigations in the field of adaptive camouflage. The overall concept is to integrate several active and passive adaptation mechanisms into a textile-based soldier camouflage system. The system should be capable of sampling and representing the background signature to adapt to different, changing backgrounds and circumstances (lighting, weather, etc.). The combination of different technologies requires the creation of a multilayer structure, in which the various devices and materials will be integrated. This is highly essential for strengthening industrial competitiveness and eventually the survivability of the soldier.

The Institute also offers a wide range of services:

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

Investigation of the thermal properties of spacer fabrics with bio-ceramic additives experimentally and using the finite element model

The heat resistance of fabric enhanced by bio-ceramic additives (BCAs) is investigated theoretically and experimentally in order to determine the influence of modification of the infrared (IR) absorption property of fabric. The enhanced IR sensitivity of textiles improves the thermoregulatory processes when worn in cold environments. The finite element model has been developed by taking into account the coupled phenomena of heat conduction, surface convection and the interaction of the fabric with IR power flux by employing heat transfer differential equations and the Stefan-Boltzmann law. Evaluations of IR absorptivity, reflectivity and transmissivity, the temperature transients during the hot plate chamber test and heat retaining properties of the fabric heated by an IR lamp have been obtained experimentally and simulated using the developed finite element model. The values of model parameters have been found, which provided a satisfactory match between the computation and the experiment in all considered cases. Simultaneously, the obtained values were reasonably close to rough theoretical estimations. Efforts have been made to distinguish from each other the influence of diffusive and radiative components of heat transfer, which affect the results of thermal resistance tests. The comparative analysis of contributions of different heat exchange mechanisms allows a better understanding of the peculiarities of standard heat resistance measurement procedures applied to BCA-enhanced fabrics and facilitates the validation of the computation models.

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Development and characterisation of microwave shielding fabrics with conductive polymer coatings

Investigation of designed electrically conductive fabrics with low surface resistivity, coated with a formulation containing the conjugated polymer system poly(3,4-ethylene-dioxythiophene)-polystyrene sulphonate (PEDOT-PSS), was performed. Different coatings with various patterns and different coating deposits were examined. Methods for measurement of electrostatic properties, reflection and transmission, were used for the characterisation. The electromagnetic radiation (EMR) shielding effectiveness was evaluated. The EMR shielding properties were investigated within 2–12 GHz frequency range. The influence of distribution and deposit of conductive coating on shielding effectiveness (SE) of textiles was determined. The optimal coating deposit ensuring the satisfactory SE of 20 dB was obtained (Fig. 3). The correlation between SE and electrostatic properties of developed coated fabrics was evaluated as well. It was found that fabric coated with the composition of PEDOT-PSS polymer dispersion pasta has EMR shielding advantage concerning earlier developed fabric with metalised yarns. Shielding properties of coated fabrics were steady in all tested range of 2–12 GHz. The values of surface conductivity σ_s , calculated taking reflection and transmission measurements into account, strongly correlate with SE. This makes it possible to distinguish the fabrics with a different coating deposit, a task that was complicated to perform using electrostatic parameters.

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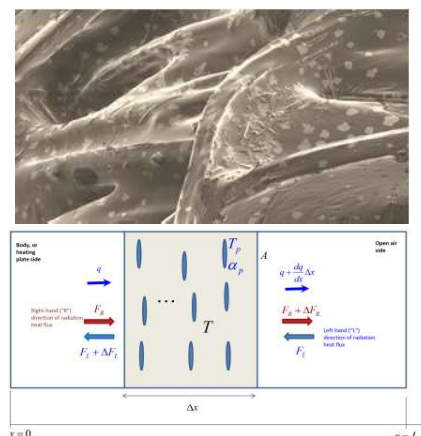


Fig 1. SEM-image of BCA zones (Ti ceramic containing printing paste), magnification 1000x and a scheme of the mathematical model of coupled diffusive and FIR heat exchange within a differential element of the fabric with BCA.

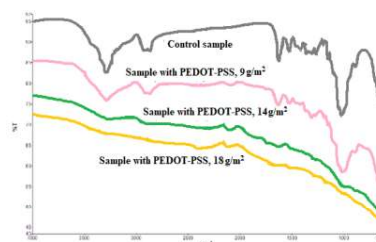


Fig. 2. FTIR ATR spectra of the control sample and samples fully coated with PEDOT-PSS.



Fig. 3. SEM-image of a sample with an optimal coating deposit.

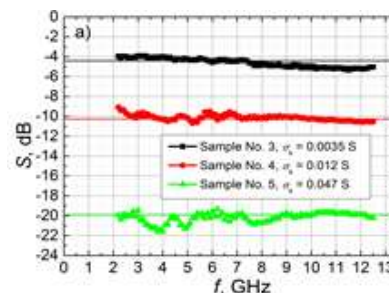


Fig. 4. Shielding effectiveness of the fabrics coated with PEDOT-PSS.



Technology innovations

Model of an intelligent heating textile product

The model of an intelligent clothing product, ensuring a comfortable microclimate to the user with two heating elements on the back, was created. The offered model has flexible and soft heating elements that are manufactured from 100% of textile materials. The heating elements are resistant to moisture and water and withstand care procedures, such as machine wash. The temperature distribution on the element is significantly more effective than on those with the wires used in the heating element. To provide the electrical conductivity of the heating element, the silver (Ag)-plated polyester yarns are incorporated in the backside of the new knitted structure. Heating textile can be used as a protective wearing in low-temperature environments, as intelligent sportswear, for disabled people, and in medical and military products.

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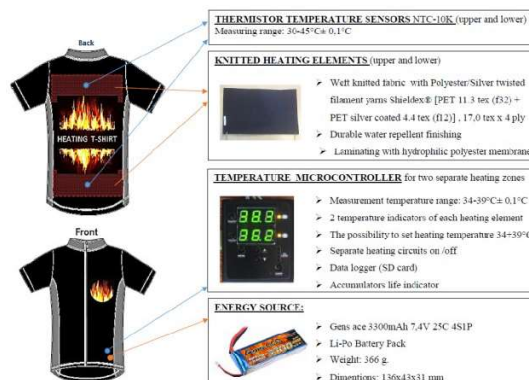


Fig. 1. Components of a model of an intelligent heating textile product.

CMR-B-scalar magnetic field meter

The CMR-B-scalar-06 is a handheld magnetic field meter which detects and measures the magnitude of magnetic field induction of pulsed, slow alternating or permanent magnetic fields in the range 0.1- 10 T. The measurement frequency ranges from DC to 100 kHz. The CMR-B-scalar-06 consists of a handheld magnetic field meter and a probe (flexible or semi-flexible) containing a memory chip for the collection of calibration data. The operation of the meter is fast and can be easily adapted to different measuring tasks. The meter has an electronic circuit with a touch screen multi-colour graphical display and a micro SD memory card for data storage. Available for the market. EU and LT patents granted.

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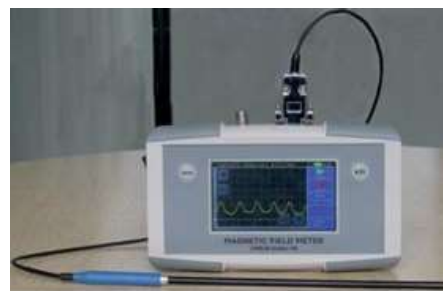


Fig. 2. The external view of the CMR-B-scalar-06 magnetic field meter.

Compact high-sensitivity potentiometer for detection of low ion concentrations in liquids

The compact potentiometer, based on an electronic circuit protected from electrostatic and electromagnetic interference, was developed for the measurement of low ion concentrations in liquids. The electronic circuit of the potentiometer, consisting of analogous and digital parts, enables the measurement of currents at the fA level. As a result, it is possible to perform reliable measurements of ion concentrations in liquids as small as 10^{-8} - 10^{-7} M. The instrument was tested by using electrodes that were selective for tetraphenylphosphonium (TPP+) ions. The characteristic response time of the potentiometer electronic circuit to changes in the concentration of these ions in a liquid is of the order of 10 s. The investigation of TPP+ absorption by baker yeast has shown that this device can be successfully used for the long-term (several hours) measurements with zero signal drift, which was about 1 μ V/s. Due to small dimensions of the electronic circuit (7.5×2×1.5 cm), this potentiometer can be easily installed in a large apparatus in the laboratory conditions (≈ 25 °C), e. g. in high pulsed magnetic fields generators that are used in electroporation studies of biological cells.

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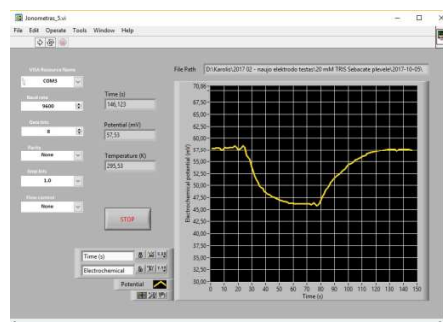


Fig. 3. (top) The external view of the ion selective electrode (a) and the potentiometer (b) used for TPP+ ion detection. The scale unit on the (a) corresponds to 4 mm. (bottom) The window software of the potentiometer used for the detection of low ions concentration in liquids.

Antibacterial coating of aluminium foil

Our technology envisages the widening of fields, where the aluminium foils can be successfully used as fresh foods package material with uniformly coloured extremely thin, $\text{ca} < 1.0 \mu\text{m}$, anodic film. This technology was discovered for fabrication of very thin and flexible anodic film with encapsulated silver nano-species on the surface of commercial aluminium foils. The results obtained from in vitro tests indicated that as-formed Ag-in-alumina films, containing $\geq 19 \mu\text{g cm}^{-2}$ of silver, possess antimicrobial properties. These films can be used as promising food packaging material. The coatings are crush-resistant during the packaging.

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Bessel-like beam generation

Microaxicons are optical elements for Bessel beam applications in microscopic scale (e. g. trapping of particles or cells) due to integrability and low weight. Here, we demonstrate an easy, fast and flexible method to fabricate microaxicon-like elements over a large area based on the four-beam interference lithography and investigate the influence of geometrical parameters of microaxicon-like structures to the Bessel-like beam formation.

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Chitosan-graphene oxide Riboflavin biosensor

Our biosensor technology employs riboflavin, also known as vitamin B2, for detecting of some biologically active compounds in foods and other solubles. Polymerised riboflavin is of natural origin and together with chitosan provides a biocompatible environment to labile proteins. We developed a lithographically miniaturised sensor manufacturing to create efficient, simple and easy to manufacture electrochemical biosensors. The technology decreases total cost by requiring only very low quantities of expensive reagents. It also increases sensitivity and permits parallel biorecognition. Our biosensor is developed to detect two main important compounds – monosodium glutamate (E621) and hypoxanthine. Monosodium glutamate is an essential amino acid responsible for unique flavour properties – the fifth taste sense – umami. Hypoxanthine is a degradation product of purines, by its oxidation to uric acid. The abnormal degradation, thus high levels of uric acid in blood and urine, can result in clinical conditions such as renal failure, gout, motor dysfunctions, etc. Moreover, hypoxanthine levels are tied to the evaluation of meat freshness, especially of fish and its products. The polymerised riboflavin biosensors can electrochemically detect amino acids in real food samples, i.e. tomato ketchup. The glutamate micro biosensor shows extremely high sensitivity of $16 \text{ mA/ mmol L}^{-1}$ for monosodium glutamate and $803 \mu\text{A/ mmol L}^{-1}$ for hypoxanthine.

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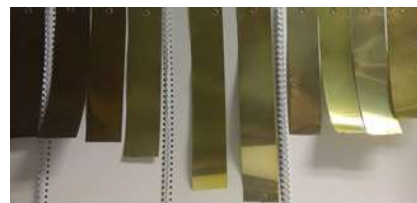


Fig. 4. Samples of aluminium foil with an antibacterial coating. Colour changes from darker to lighter as the layer gets thinner.

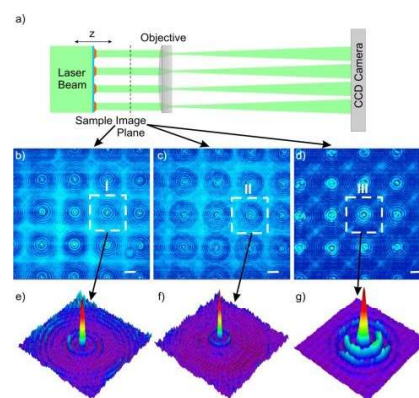


Fig. 5. Example of fabrication of microaxicon-like elements over a large area based on the four-beam interference lithography.



Fig. 6. The external view of the Riboflavin biosensors.

Technology for selective metal deposition on dielectric materials

Fabrication of circuit traces is the most challenging task in Moulded interconnect devices (MID) production, being both technically difficult to achieve and challenging to make cost-effectively. Moulded interconnect devices (MID) – an injection-moulded thermoplastic part with integrated electronics – offers material, weight and cost savings by integrating electronic circuits directly into polymeric components. The Selective Surface Activation Induced by Laser (SSAIL) is a new patent-pending technology for writing electronic circuits directly onto the dielectric material by modifying surface properties with a laser and electroless chemical deposition has been developed at FTMC. Lasers can write the circuits directly by modifying the surface of polymers followed by an electroless metal plating. The new technology offers laser writing speeds of up to 4 m/s, and spatial plating pitch is kept narrow at 25 μm for polymers and less than 10 μm for glass substrate. SSAIL is cost-effective technology comparing with state of the art currently used in industry – Laser Direct Structuring (LDS) and is capable metalise not only on opaque polymers but also glass and transparent polymers. The real demonstration has been fabricated in collaboration with Fiat Research Center (Fig 7). Feasibility of the technology have been shown by LED matrix demonstrator on glass (Fig. 8) and transparent polymer (Fig.9). Applicable substrates: polymers – polycarbonate (PC), acrylonitrile butadiene styrene (ABS), polyamide (PA), polyvinyl chloride (PVC), polyphthalamide (PA), polyether ether ketone (PEEK), liquid crystal polymer (LCP), ABS for 3D printing, polyethylene terephthalate (PET), polyimide (PA). Glass – soda lime, float glass, Fused silica. Potential market: embedded electronics for automotive and consumer products, etc.

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Flow process application in Suzuki reaction

Suzuki reaction is used in the synthesis of biaryls from halides and boronic acids in the presence of palladium catalysts. The removal and recycling of soluble salts and microparticles of palladium after the reaction remain a serious task. Another problem is the use of environmentally toxic solvents like toluene and dioxane. We have first experimental data about the possibility to perform the coupling of aryl boronic acid and aryl halide in alcohol/water solutions using immobilised palladium catalyst. The yield of reaction reaches 98% and better, and the product isolation in 98% purity can be achieved by dilution of the reaction mixture with water. Reaction and workup require smaller volumes. Multiple uses and full recycling of palladium catalyst, also partial recycling of alcohol is possible. Potential market: materials and electronics manufacturing, working environment and safety improvement. A new process might be used in the synthesis of intermediates for energy harvesting and another material.

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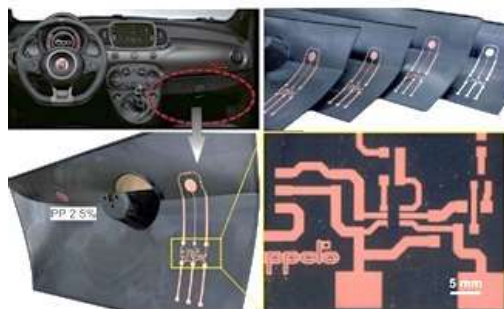


Fig. 7. Example of laser-based selective metalisation technology application on various plastics.

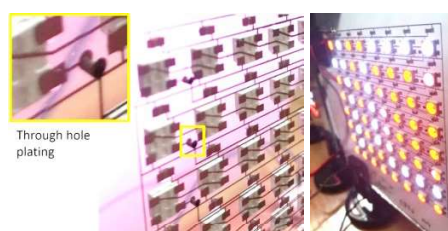


Fig. 8. Demonstrators on a glass substrate.
a) LED display matrix 8x8 with the circuit fabricated on both sides of the glass substrate.

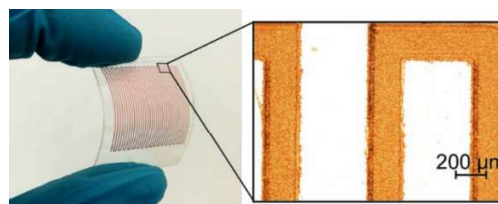


Fig. 9. A flexible transparent PET with a circuit pattern made by SSAIL.



Fig. 10. Hybrid flow reactor prototype for Suzuki reaction.

Calliper with laser healing

The prototype is a low-level laser therapy (LLLT) device which uses pulse laser radiation incorporated in the calliper. The pulsed laser probe gives clinicians the ability to deliver more energy, deeper and faster than any other probe, providing the power necessary to treat deeper musculoskeletal conditions, fractures and deep-seated pain. LLLT may be administered by physicians, physical therapists or occupational therapists. It could be used in an outpatient setting with no anaesthesia or sedation for various diseases: wound healing, smoking cessation, tuberculosis, temporomandibular joint disorders, a variety of musculoskeletal conditions that include carpal tunnel syndrome, fibromyalgia, osteoarthritis, rheumatoid arthritis.

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Fig. 11. Calliper with laser healing prototype.

Hybrid 3D laser processing of glass for high-density capillary gas nozzles

The laser rear-side processing approach allows flexible 3D processing of glass, including cutting and free-shape milling. Example of rapid fabrication of gas jet nozzles with the minimum 100 μm -diameter capillaries in a 6.3 mm-thick fused silica are presented. The maximum material removal rate for high-volume parts is 2.34 mm^3/s with the roughness is on the order of several micrometers. The laser-assisted selective etching (FLISE) technology can significantly improve the surface roughness (~ 12 times); however, due to the low fabrication time, it is less competitive for processing of high-volume parts. The limitations above can be eliminated by the hybrid 3D machining technique, when high-volume parts, which do not require high quality, are removed by nanosecond pulses, and high-quality capillaries are fabricated by the laser-assisted chemical etching. Such a technique allows achieving both - high processing speed and quality.

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Fig. 12. The nozzle (35 mm-diameter, 12 mm-height) with a 2 mm-length channel with the output diameter of 100 μm , machined in fused silica combining the rear-side laser processing and laser-assisted selective etching technology, and optical element with laser cut hole.

3D laser milling

Ultrashort laser pulses have many applications due to the possibility of precise material removal (ablation). The additive manufacturing of three-dimensional (3D) objects is the high interest of industrial end users. FTMC has developed 3D laser milling technology which competes with traditional CNC milling when micrometre precision is required. New technology offers ultra-efficient, high-quality, contactless, and heat-affected-zone free engraving of 3D objects by utilising laser irradiation with milling rates up to 6 mm^3/min .

Potential market: micro-mould fabrication for plastics.

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Fig. 13. 3D Albert Einstein's face profile milled by a picosecond laser in bulk copper, dimensions 10×10×2 mm^3 .

Open access centers

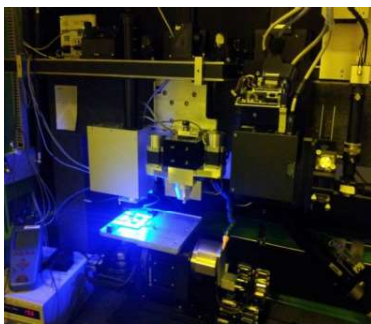


OAC for electron microscopy, X-ray diffractometry and spectrometry

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: 1) Laser processing: in-Glass marking; laser beam interference ablation; laser direct writing; ultrashort pulse laser ablation. 2) Molecular: dip pen nanolithography; microcontact printing; piezoelectric inkjet printing; colloidal nanolithography. 3) 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.



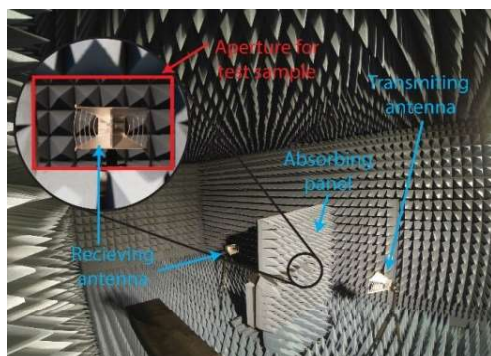
OAC for converse and chemical coatings

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 Physical 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.



OAC for prototype formation and integration

Clean room technology for prototyping of semiconductor based devices

Based on a collaboration between the Departments for Physical Technologies and Optoelectronics, a complete cycle of the clean room (CR) microprocessing line has started to function. It 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 the 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: 1) CR (ISO7–ISO5 about 300 m²) operations, 2) photolithography, 3) laser lithography, 4) wet chemical processing, 5) thermal processing, 6) metal and oxide coatings, 7) 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 the laboratory (TRL 4) or relevant environment (TRL 5), and up to demonstration in a relevant environment (TRL 6). In specific cases, collaboration can reach prototyping in an operational environment (TRL 7). For this, we use the methods acceptable to characterise the components and devices at the nanometer scale level and the level of the complete unit.

The characterization includes: 1) topography, force spectroscopy, tunneling current spectroscopy by scanning probe microscopy, 2) standard I-V and C-V characteristics in the dc- and ac-modes by the probe station, 3) photovoltaic parameters with the A1.5 solar source by special set-up, 4) gas response in the synthetic atmosphere under strictly controlled conditions by gas flow control system. We also carry out special set of tests to determine the response and resistivity to the microwave irradiation.

Metrology



National metrology institute of Lithuania

A one-inch error at the start can be a thousand miles at the end (Chinese proverb)

Department of Metrology (DM) was authorized to perform and implement functions of the National Metrology Institute (NMI) since 1 July 2014. Year 2018 was historical for metrologists all over the world. BIPM's Member States voted on 16 November 2018 to revise the International System of Units (SI), changing the world's definition of the kilogram, the ampere, the Kelvin and the mole. Two researchers from DM were authorized by the Decree of Prime Minister of Lithuania to represent our country during the 26th General Conference on Weights and Measures (CGPM) in Versailles, France.

DM maintains national standards in five different measurement fields. **Time and Frequency Standard Laboratory (TFSL)** is reproducing values of the unit of time, the second (s) and the unit of frequency - hertz (Hz). Its mission is representation of Lithuanian Coordinated Universal Time UTC(LT), 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 TFSL in cooperation with the JSC "BaltStamp", provides time stamping services, which meet the eIDAS regulations. Also, in cooperation with the Swiss company "GVR Trade" and the Lithuanian JSC "MitSoft", the TFSL pursue the EUROSTARS-2 project entitled „System of passive SAW sensors exploiting UWB hyperbolically frequency modulated Signals“ (UWB_SENS).

The mission of the **Electrical Standards Laboratory (ESL)** is maintaining and developing the standards of unit of voltage, the volt (V), and unit of resistance, the ohm (Ω), ensuring their traceability to the SI, calibrating working standards and measurement devices, pursuing research in the field of measurement of voltage, resistance and electrical current.





The mission of the **Temperature Unit Standard Laboratory (TUSL)** is realising the international temperature scale ITS-90 and the value of the unit of temperature, the Kelvin (K), and ensuring their traceability to SI. Lithuanian national standard of the temperature unit in the range from -195°C to +961.78°C is of primary level and +1084.62 °C reference point (freezing point of Cu) is of the secondary level.

Metrology is not restricted only to standards of physical units. The **Laboratory for Metrology in Chemistry (LMiC)** provides reliable and accurate chemical measurements in sectors of health care, food safety and environmental protection. In the framework of the European Metrology Programme for Innovation and Research (EMPIR), the laboratory participated in the ALCOREF Project „Certified forensic alcohol reference materials“. The consortium of 10 partners from 10 different countries was formed with the coordination of the Federal Institute for Materials Research and Testing (BAM, Germany). The main objectives of the project are research of accurate measurements, homogeneity, short- and long-term stability for certification of ethanol/water certified reference materials and new regional metrological capacity for breath alcohol control.



Fig. 1. Project partners and ALCOREF project kick-off meeting, 16th - 18th October 2017 in BAM (Berlin, Germany)

The **Ionizing Radiation Metrology Laboratory (IRML)** is piloting the EURAMET Project No. 1437 “The follow-up interlaboratory comparison of the radionuclide calibrators”. The secondary standard equipment for radionuclide measurement in a high activity range (above 1 MBq) used in Lithuania was compared with the similar equipment used in the Czech Republic and Slovakia. The radionuclides applied in nuclear medicine, such as ^{18}F , ^{67}Ga , ^{99}Tc , ^{111}In , ^{123}I , ^{125}I , ^{131}I , ^{137}Cs (as a check source), ^{201}Tl and ^{223}Ra , have been standardised with the well-type ionising chambers Fidelis and Capintec 15R, the uncertainty budget was evaluated. The results confirmed that consistent, safe and effective radionuclide activity measurement services to the medical community are provided in Lithuania.

Investigation of the thermal properties of spacer fabrics with bio-ceramic additives experimentally and using the finite element model

The heat transients during the hot plate chamber test and heat retaining properties of the fabric of contributions of different heat exchange mechanisms allows a better understanding of the peculiarities of standard heat resistance measurement procedures applied to BCA-enhanced fabrics and facilitates the validation of the computation models.

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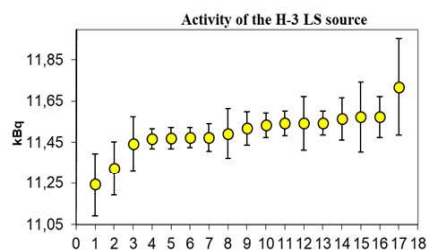
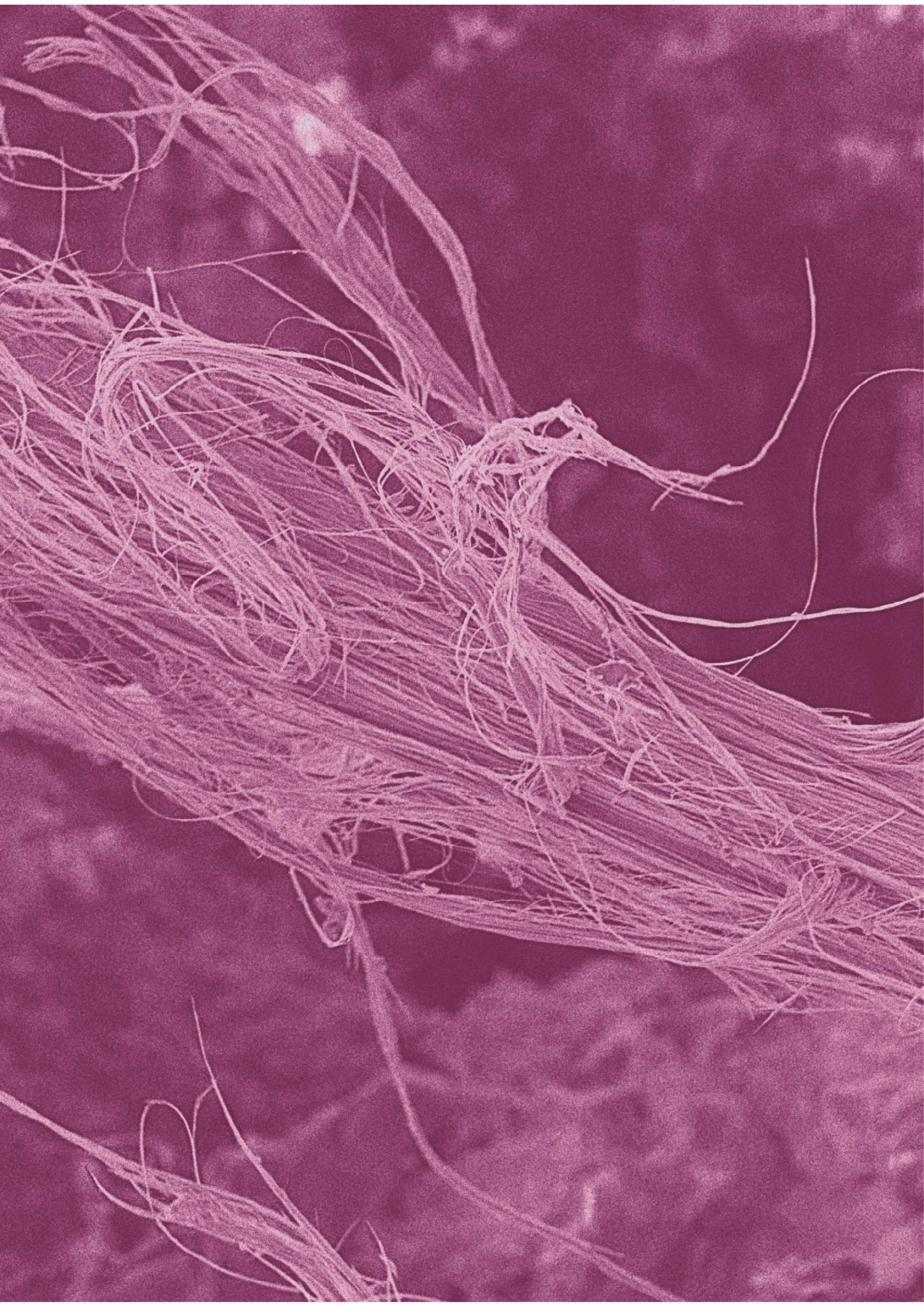
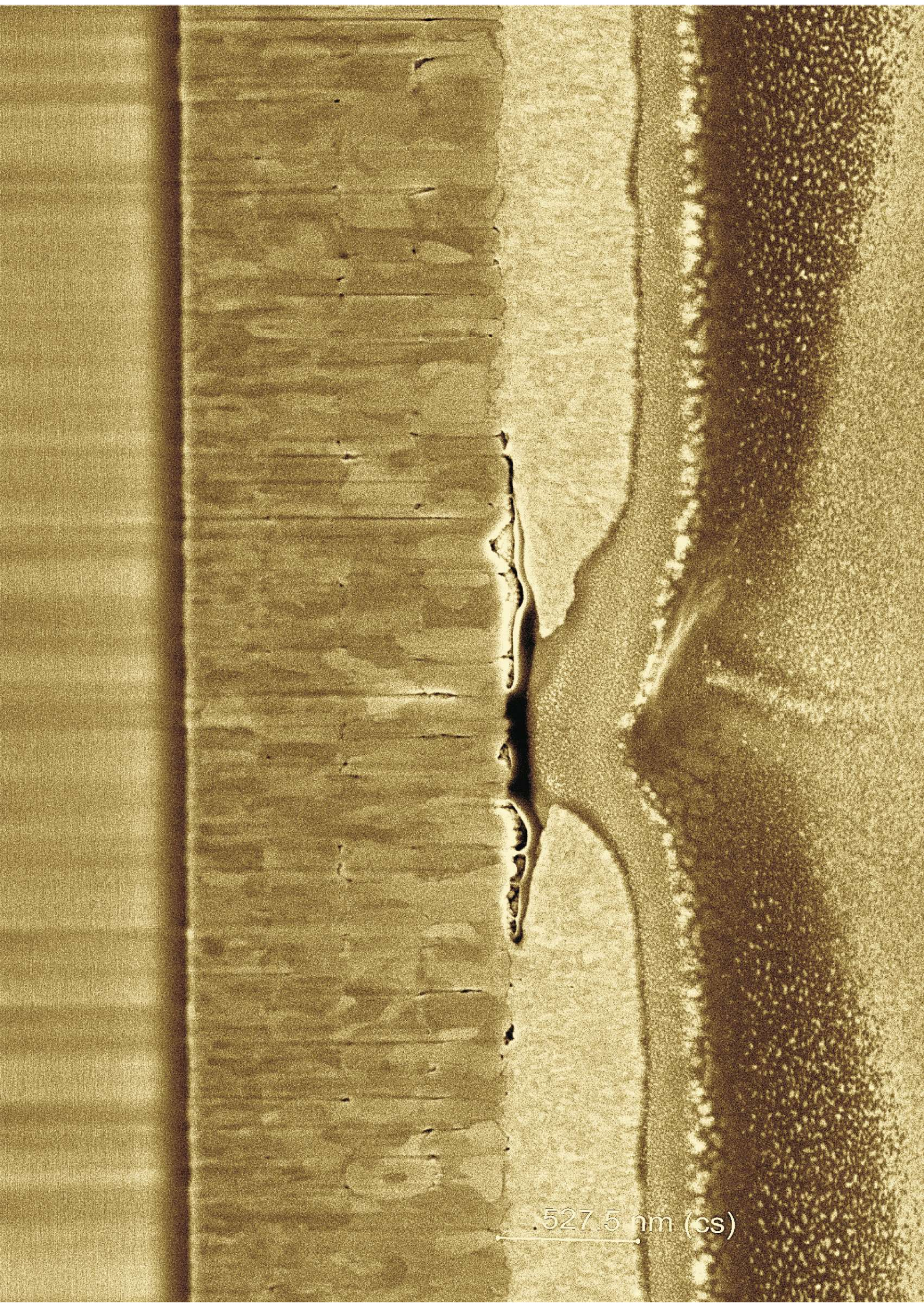
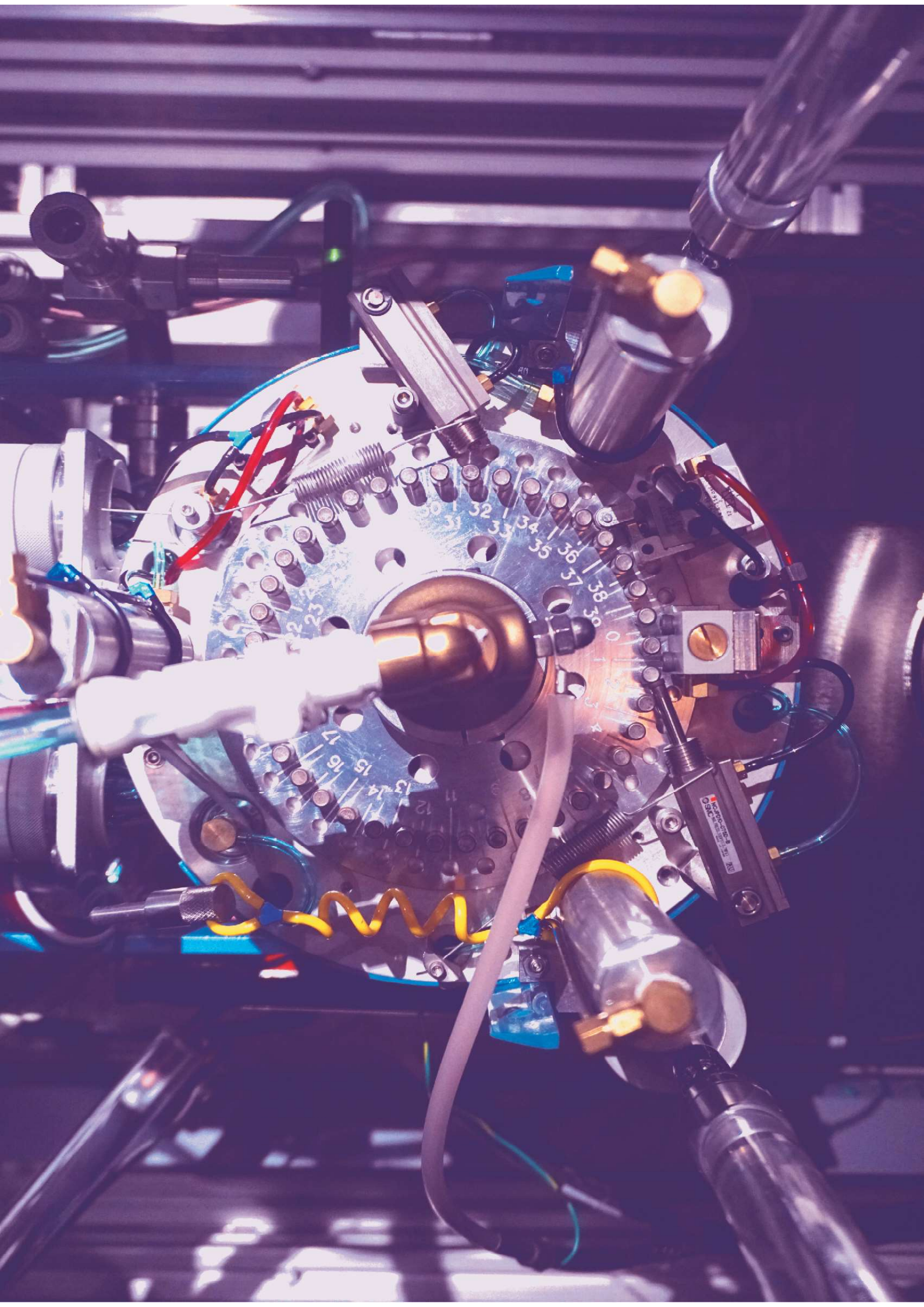


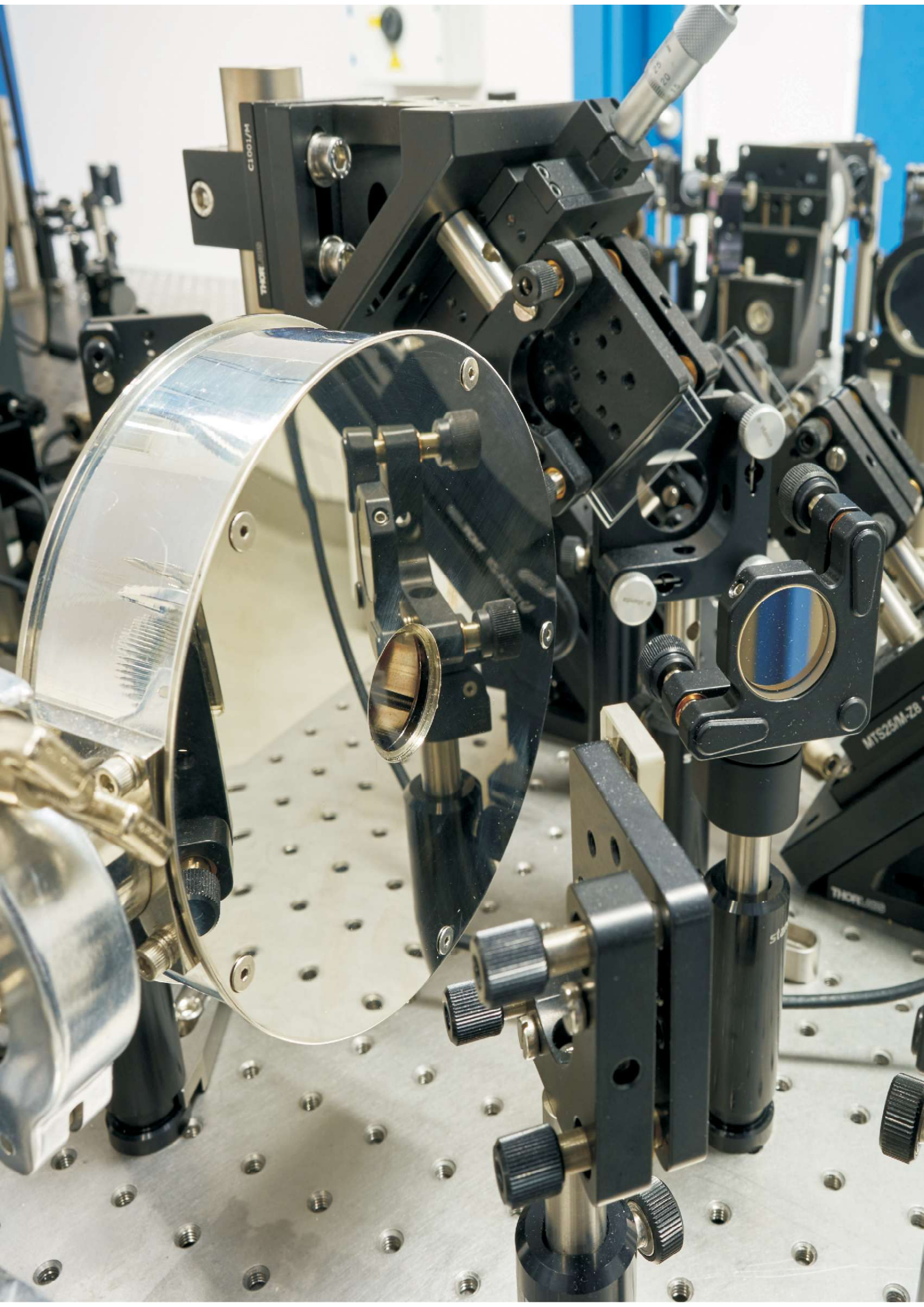
Fig. 1. Results of the comparison CCRI(II)-S12.H-3. The number on the x-axis corresponds to participating laboratories, FTMC is No 11.





.527.5 nm (cs)







Projects

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

European Commission 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

Research Executive Agency (REA), delegated by the European Commission project "Graphene-Manganite nanostructures for novel pulsed magnetic field sensors" (GRAMAS)

R. Lukošė

European Space Agency (ESA) project "IntraRed Bismuth-based Sources" (IRBIS)

R. Butkutė

Research Executive Agency (REA) project "A multi-spectroscopic approach to probe amyloid aggregation at biological surfaces" (MultiSpecAMYLOID)

S. Strazdaite

European Space Agency (ESA) project "Directive transistor-based THz detectors" (THzFET)

I. Kašalynas

European Defence Agency (EDA) project "Adaptive Camouflage for the Soldier II" (ACAMSII)

A. Abraitienė

European Commission project "Advancing Science and Technology through diamond Quantum Sensing" (ASTERIQS)

A. Alkauskas

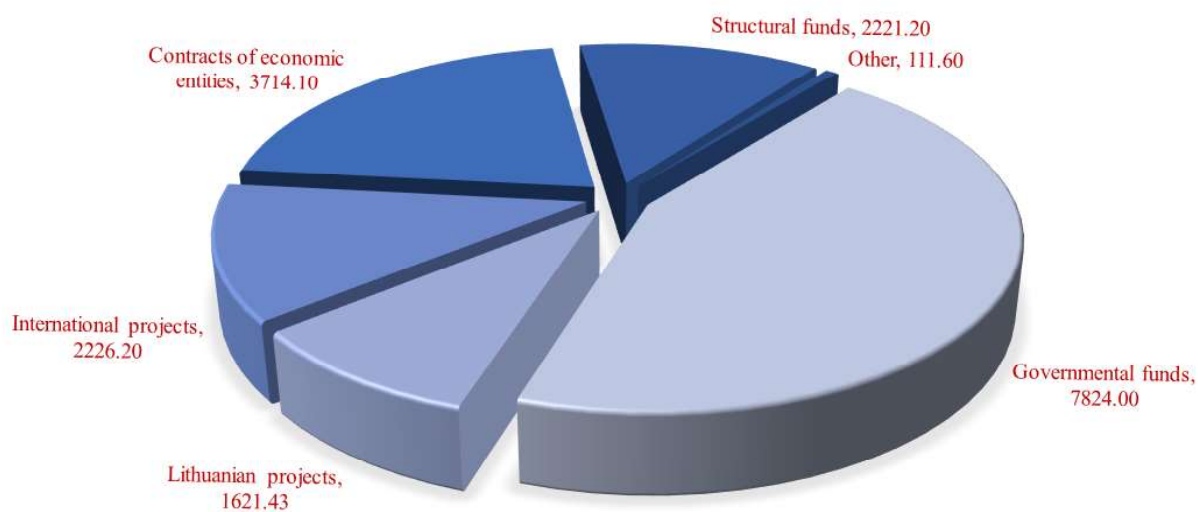




Structure and statistics

SCIENTIFIC BOARD	DIRECTOR	INTERNATIONAL ADVISORY BOARD
Department of Chemical Technologies	Department of Environmental Research	ADMINISTRATION
Department of Electrochemical Materials Science	Department of Nuclear Research	DOCUMENT MANAGEMENT DEPARTMENT
Department of Catalysis	Department of Laser Technologies	DEPARTMENT OF INTERNAL AUDIT
Department of Characterization of Materials Structure	Department of Molecular Compound Physics	DEPARTMENT OF ECONOMICS AND PUBLIC PROCUREMENT
Department of Organic Chemistry	Department of Nanoengineering	DEPARTMENT OF INNOVATION AND TECHNOLOGY
Department of Electronics	Industrial Laboratory for Photonic Technologies	DEPARTMENT OF SCIENTIFIC TECHNICAL INFORMATION
Department of Physical Technologies	Department of Textile Technologies	DEPARTMENT OF FINANCES
Department of Fundamental Research	Accredited Department of Textiles Physical – Chemical Testing	DEPARTMENT OF LAW AND PERSONNEL
Department of Material Science and Electrical Engineering	Department of Textile Product's Technological Development	DEPARTMENT OF DOCTORAL STUDIES
Department of Optoelectronics	Department of Metrology	MAINTENANCE DEPARTMENT

Budget of FTMC 2018, kEur





Events

GUESTS FROM CHINA

/2018 01 21/



In the framework of the program prepared by the Lithuanian Laser Association, the group of scientists from the Center of Laser Research, the Institute of Oceanography Equipment and the Academy of Information and Communication Technology of Shandong Academy of Sciences, China visited the Department of Optoelectronics of FTMC and was acquainted with the activities of our Center.

SWEDISH SCIENTISTS “DISCOVER” FTMC

/2018 02 26/



The series of seminars, moderated by Arūnas Krotkus, head of the Department of Optoelectronics, were given by guests from Linköping University, Carlito Ponseca, Olle Inganaes and Feng Gao.

TOPICAL MEETING ON ELECTROCHEMISTRY

/2018 05 08-11/



The FTMC co-organised 23rd Topical Meeting of the International Society of Electrochemistry (ISE) „Electrochemistry for Investigation of Biological Objects: from Functional Nanomaterials to Micro/Nano-Electrodes“. The meeting brought 100 leading bioelectrochemists from all over the world. The participants presented their research and visited the laboratories of FTMC and Life Sciences Center. Two former presidents of ISE were awarded the Theodor Grotthuss' medals during the Gala dinner of the Conference.

GUESTS FROM UNITED ARAB EMIRATES

/2018 05 10/



The business delegation and the accredited ambassador to Lithuania Yousif Eisa Hassa Eisa AlSabri were the guests of the Laser and Engineering Technology cluster (LITEKTM). The aim of the visit was to activate the cross-border cooperation by getting the knowledge of the traditional industry and agriculture, as well as on high technologies in Lithuania. The delegation visited the laboratories of LITEKTM, was acquainted with the development of the 3D printing technologies and the construction of high-power laser systems. The director of FTMC, G. Valušis, shared the experience of FTMC on setting-up technological enterprises in the field of photonics, emphasising the importance of research in optoelectronics for the development of innovative industry in Lithuania.

QuEBS CONFERENCE

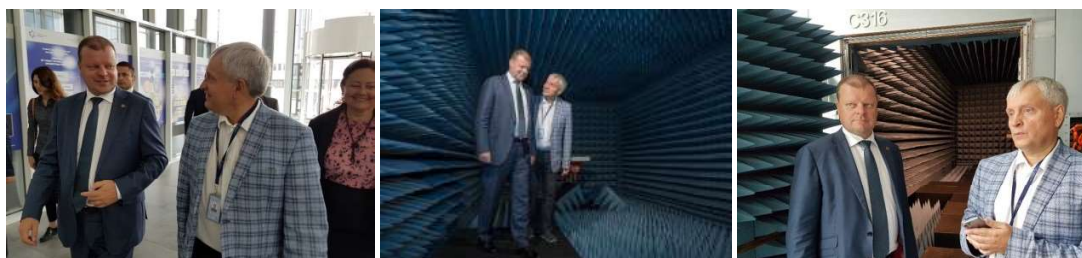
/2018 07 10-13/



A rather new field of science—quantum biology was for the first time represented in Lithuania. The founders of this field, as well as possible Nobel prize candidates, were among the presenters of the QuEBS conference. „The competition to organise the conference was very tough, and we are happy to be honoured“, told one of the organisers, the head of the Department of Molecular Compound Physics of FTMC Leonas Valkūnas. There were plenty of great names in this conference: Graham R. Fleming, Shaul Mukamel, Rienk van Grondelle and some others. The presentations were also given by the scientists from FTMC Jevgenij Chmeliov, Andrius Gelžinis and Marijonas Tutkus.

PRIME MINISTER SAULIUS SKVERNELIS VISITS FTMC

/2018 08 14/



FTMC director Gintaras Valušis acquainted the Prime Minister of Lithuania with research and development activities, and future prospects of our Center. Saulius Skvernelis paid a visit to scientific laboratories equipped with modern infrastructure. „FTMC is a good example to every institution. We see now that the funds invested here give a good pay-off - the Center earns more than gets from the state. FTMC demonstrates that the most valuable commodity is our ability to capitalise intellect and knowledge“, told Saulius Skvernelis.



INTERNATIONAL CONFERENCE ICPEPA

/2018 09 10-14/



International Conference on Photo-Exited Processes and Applications (ICPEPA) is a platform for the best laser technology professionals (scientists, technology enterprises, etc.) from all over the world. The conference, which started in 1993, is organised each time in different places. In 2018, Vilnius and FTMC hosted the 11th conference. It attracted more than 230 specialists (with 163 presentations) from 26 countries. The participants also had the chance to visit main laser enterprises of Lithuania. The mayor of Vilnius Remigijus Šimašius once expressed the wish for Vilnius to become the world-capital of lasers. „ICPEPA is the first real step for such a wish to become a reality“, told Gediminas Račiukaitis, the organiser of ICPEPA in Lithuania, head of the Department of Laser Technologies of FTMC.

INTERNATIONAL CONFERENCE APROPOS 16

/2018 10 10-12/



“We see the unique collaboration of science and high technologies in Lithuania”. Such was the decision of photonic science leaders after participation in the conference APROPOS 16 organised by FTMC in Vilnius. Along with the scientific sessions, the participants visited the Lithuanian laser and semiconductor enterprises („Ekspla“, „Light Conversion“ and „Brolis Semiconductors“), the FTMC Technology Park and the laboratories of FTMC. The conference has a very long tradition. It was started in 1971 as the „Plasma and Instabilities“ symposium. At that time, it was organised by the Institute of Semiconductor Physics, one of the leaders in this field of physics. From 1992 the conference turned its attention to ultrafast processes in semiconductors. The main focus of APROPOS 16 was the problems and challenges of photonic and modern optoelectronic materials and devices.

FTMC CONFERENCE FOR PHD STUDENTS AND YOUNG SCIENTISTS

/2018 10 17-18/



Young scientists presented the results of their research in physics, chemistry, material science and engineering. The participants were welcomed by the director of FTMC Gintaras Valušis. The PhD students had the possibility to discuss



not only scientific but also psychological problems they encounter during their studies. One session was devoted to invited lecture “Stress during PhD: friend or enemy?” of Ieva Vasionytė, the psychologist from Vilnius University.

IUPAP MEETING IN FTMC

/2018 10 31-11 02/



The meeting of the International Union of Pure and Applied Physics (IUPAP) for the first time was held in Lithuania. Created in 1922 in Belgium and now residing in Singapore, the organisation unifies the scientists from more than 60 countries. IUPAP is interested in problems of fundamental and applied physics, international collaboration and promotion of physics. Lithuania entered this union in 2002 and has one vote in its General Assembly. This IUPAP meeting in Vilnius was a continuation of the Laser Physics and Photonics meeting of IUPAP which was devoted to discussing the problems of photonics application.

NEW YOUNG ACADEMICIAN

/2018 12 18/



A chief research fellow of the Department of Laser Technologies, FTMC Mindaugas Gedvilas was elected a member of the Young Academy of Lithuanian Academy of Sciences. The Young Academy created in 2018 is a subdivision of LAS for active young researchers. The election is competition-based, and each year ten members are elected for a four-year term.

LEISURE LABORATORY





Awards



Arūnas Krotkus – for lifetime achievements

Arūnas started to work at Semiconductor Physics Institute – a predecessor of FTMC, after graduating Vilnius University in 1970 and was working there since then. His research interests evolutioned from hot-electron phenomena in semiconductors to ultrafast optoelectronics and ultrafast semiconductor device technology. During the last two decades his group made essential breakthroughs in epitaxial growth technology, including pioneering work on group-3 bismides, and in a terahertz frequency range physics and applications. 17 young researchers of his group have successfully completed their PhD theses; the group worked on a large number of international research projects, including 13 EU grants, and other major grants funded by NATO, ESA, and other agencies.



Svajus Asadauskas – for innovations

Along with his scientific activity, the Head of Tribology Laboratory Svajus Asadauskas transfers research findings into pilot manufacture and commercialisation. Investigations of alumina friction led to improved marine rigging rings, pistons for aviation and sports car engines, produced by FTMC startup Alanodas. Elastomer tribology studies improved devulcanization and recycling of end-of-life tires. Startup companies Rubber Products S.i.a., UAB Devulco and some others have already commercialised his devulcanization technology. Liquid lubricant R&D was recognised by two awards from InnoCentive, a world-leading research crowdsourcing platform. Thanks to the high visibility of his publications, FTMC became a significant partner in two large Horizon 2020 projects, COSMOS and TERMINUS, along with mega-companies Arkema, Bayer spinoff Covestro, TetraPak and others. His activities are an excellent example of how to produce both high impact publications and commercially-viable innovations.



Leonas Valkūnas – for scientific achievements

Leonas Valkūnas devoted many years to developing and applying the theory of exciton dynamics and relaxation in various molecular systems including artificial molecular aggregates, carbon nanotubes and photosynthetic light harvesting antenna complexes, to name a few. He created and trained a team of young, motivated researchers capable of solving the most complicated physical chemistry problems by combining the modern, multidimensional spectroscopies and elaborated theoretical modelling tools. They were able to contribute significantly into the solution of the hotly debated problems of the long-lasting coherence in photosynthetic systems. Together with colleagues, he recently published papers in Nature group journals, Journal of Physical Chemistry Letters and other prestigious journals disclosing most puzzling properties of self-regulation of photosynthetic antenna systems and whole plant leaves under varying light conditions. These publications position Leonas Valkūnas among the leaders of the field.



Aurimas Vyšniauskas – debut of the year

Aurimas Vyšniauskas has joined the Molecular Compounds Physics department after his PhD studies at Imperial College London. With a group of organic chemists and theoreticians from Vilnius University, he initiated the studies of molecular microviscosity sensors, a new research field in Lithuania. In 2018 he published three papers, including a publication in Reviews in Physical Chemistry. He has also started teaching at Vilnius University. Due to his social activity, Aurimas was elected a member of the Employees' Council of FTMC.

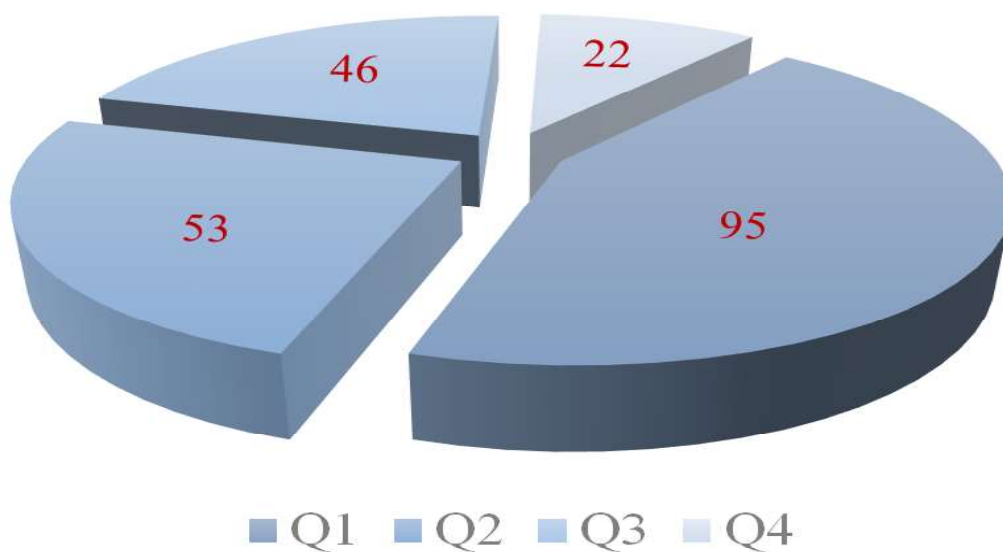


Jolanta Juodienė – for scientifically invisible activity

For her remarkable work in managing events held at the Center, for graceful acceptance of many visitors and excursions, as well as for genuine efforts in the creation of an attractive atmosphere in administration.



Publications



Publications with FTMC affiliations in 2018 in top quartile (Q1) journals

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8. Balčiauskas, Linas; Skipitytė, Raminta; Jasiulionis, Marius; Balčiauskienė, Laima; Remeikis, Vidmantas. Immediate increase in isotopic enrichment in small mammals following the expansion of a great cormorant colony // *Biogeosciences*. ISSN 1726-4170. 2018, vol. 15, p. 3883-3891.
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