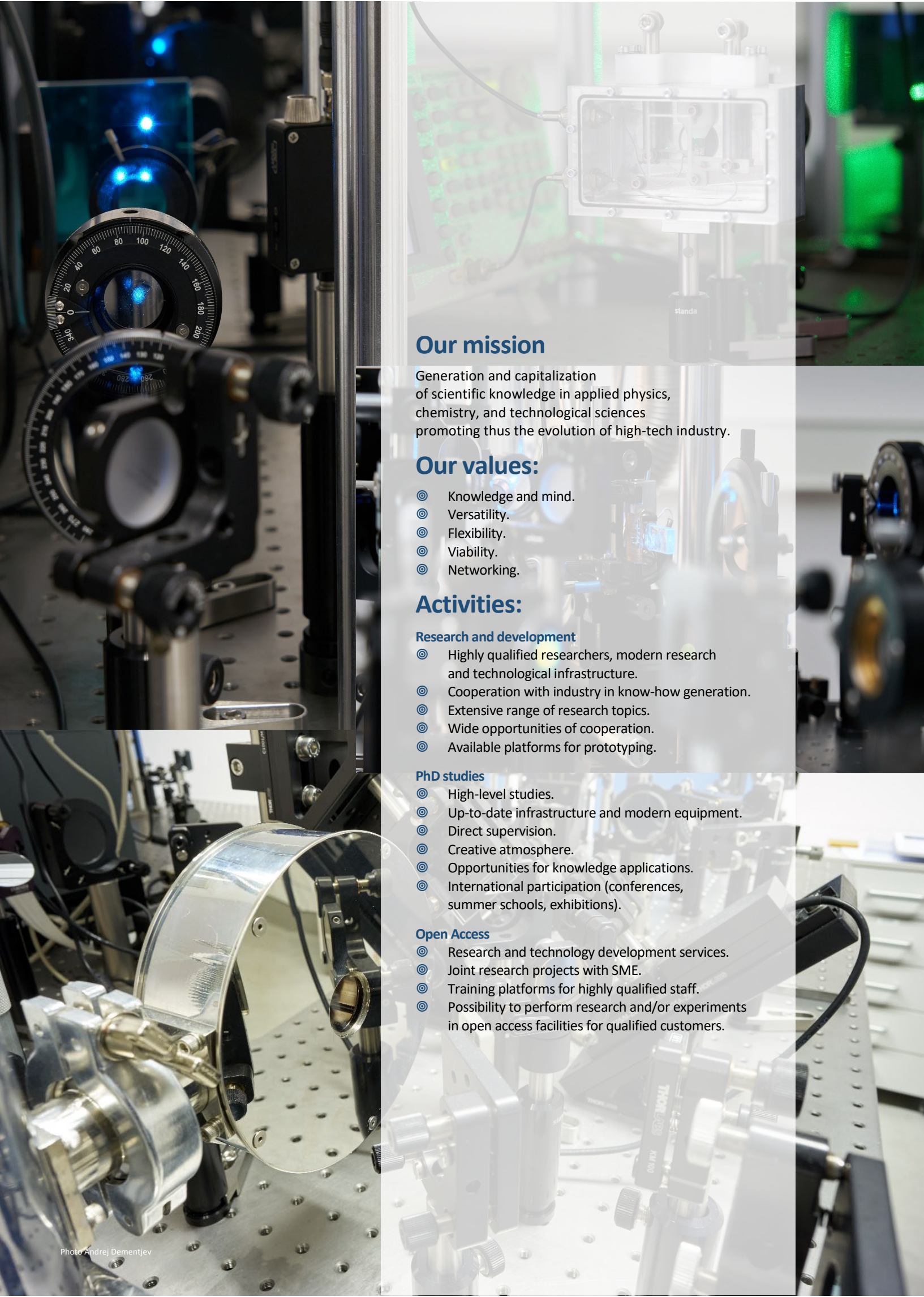


**CENTER**  
FOR PHYSICAL SCIENCES  
AND TECHNOLOGY

# Annual Report

MODERN PATHS TO INNOVATIONS  
2022





## Our mission

Generation and capitalization of scientific knowledge in applied physics, chemistry, and technological sciences promoting thus the evolution of high-tech industry.

## Our values:

- ⊙ Knowledge and mind.
- ⊙ Versatility.
- ⊙ Flexibility.
- ⊙ Viability.
- ⊙ Networking.

## Activities:

### Research and development

- ⊙ Highly qualified researchers, modern research and technological infrastructure.
- ⊙ Cooperation with industry in know-how generation.
- ⊙ Extensive range of research topics.
- ⊙ Wide opportunities of cooperation.
- ⊙ Available platforms for prototyping.

### PhD studies

- ⊙ High-level studies.
- ⊙ Up-to-date infrastructure and modern equipment.
- ⊙ Direct supervision.
- ⊙ Creative atmosphere.
- ⊙ Opportunities for knowledge applications.
- ⊙ International participation (conferences, summer schools, exhibitions).

### Open Access

- ⊙ Research and technology development services.
- ⊙ Joint research projects with SME.
- ⊙ Training platforms for highly qualified staff.
- ⊙ Possibility to perform research and/or experiments in open access facilities for qualified customers.



# Message from Director:

## A Year of 2022: Contrasts and Challenges



**The Year of 2022** was the third year of pandemics. It was **the second year** of increasing inflation and the **first year** of Russian invasion to Ukraine. These particular circumstances have imposed strong direct and indirect consequences on scientific activities of the Center for Physical Sciences and Technology (**FTMC**), stimulated a number of political and civil initiatives, introduced new discussions on development of our institution and our well-being in the face of war. It was a year of deep contrasts and high challenges, unexpected disappointments and encouraging discoveries, external uncertainties and successful solutions.

Despite all challenges and changes around, **the Year 2022 was an important step in evolution of FTMC** in scientific, innovation and project activity aspects. Scientifically, the year was thriving – of totally more than 300 international publications, more than 250 articles were published in highly-ranked scientific journals; 13 national and international patents and their applications were issued; 17 PhD students successfully defended their theses, while number of PhDs was further increasing and reached 121 currently. FTMC activity in projects writing and coordination allowed to raise their share in FTMC budget to nearly 50 percent. Despite external uncertainties and energy issues, **innovations and industry-related activities** were kept on a conventional level – the number of business clients around 400, while the number of contracts related to research and development as well as scientific services ranged up to 1000.

The year was particular in developing the relations with Taiwan scientific institutions. Together with Taiwanese colleagues, in February 2022 we have launched Taiwan and Lithuania Center for Semiconductors and Materials Science at FTMC. This Center not only covers five projects running currently, but also establishes the base for the further extensive scientific and technological links. The cooperation was enriched by several visits from different universities and Government as well as numerous delegation from the Industrial Technology Research Institute (ITRI).

**Phenomenon of patronage** which elegantly manifested itself during the Jubilee Event in 2020 was successfully continued also in the **Year 2022 – Marius Jakulis Jason Foundation** awarded grants for three talented Lithuanian scientists to return from foreign institutions; the support was also given for Ukrainian scientist working at FTMC.

We believe that the key to everyone's success and institution permanent growth is in strong motivation, personal initiatives and coherently focused activities. We intend to join our people together through our culture and values – scientific excellence, versatility and flexibility, knowledge and mind, effectiveness and networking. They are central to creating productive and attractive workplaces at FTMC dedicated to stimulate inexhaustible impetus to investigate, being passionate and making progress in whatever form of activity it takes.

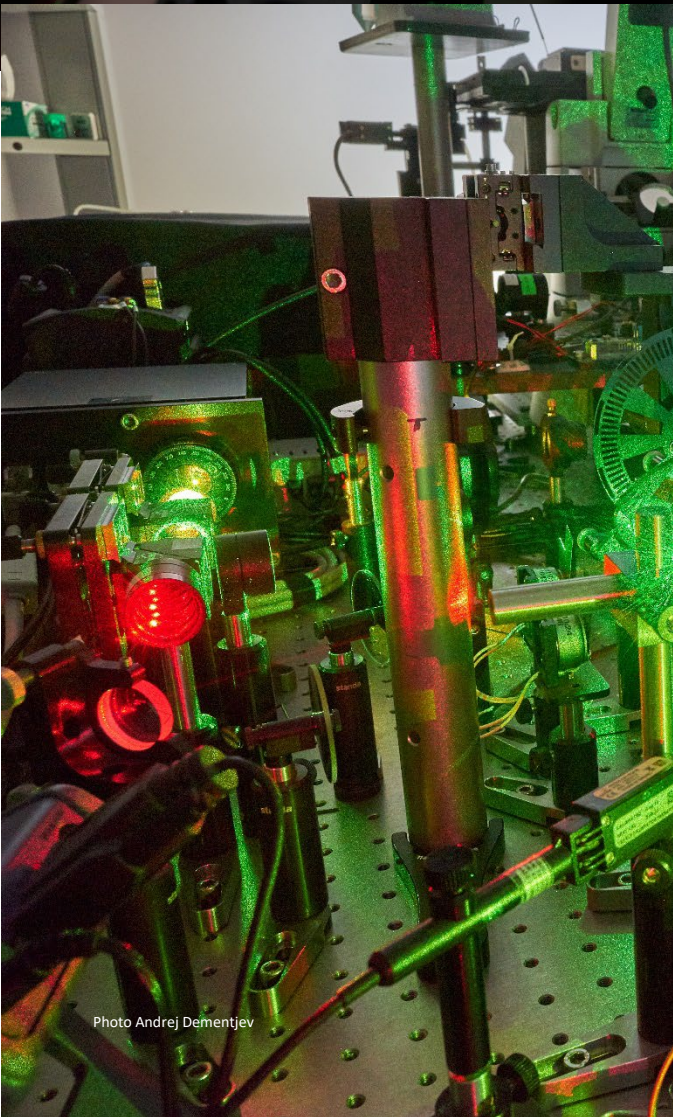
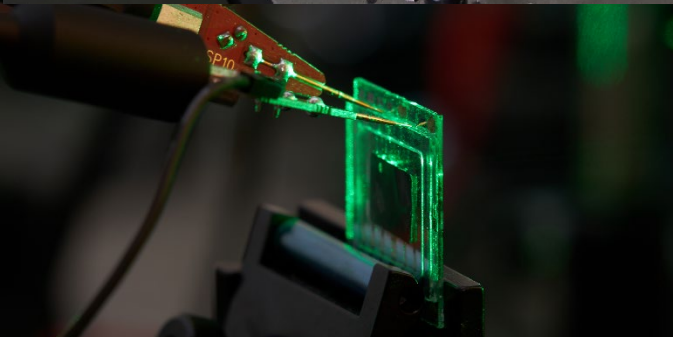
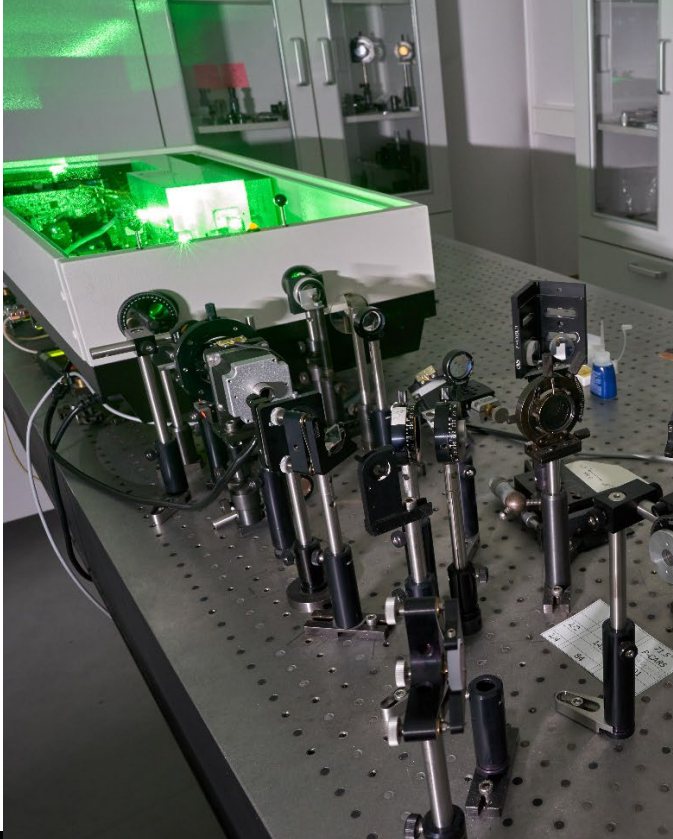
My sincere thanks to all the staff and PhD students, alumni and our friends, who continue to fulfil our mission by contributing to society through scientific research and learning, generation of intellectual property and implementation of high-tech innovations, capitalization of gained scientific knowledge and technological developments.

The **Annual Report 2022** reflecting the main scientific and technological achievements, progress in high-tech innovations as well as the most important events are presented in pages that begin here.

**Gintaras Valušis**

Vilnius, January 2023





## Scientific divisions

Department of Catalysis

Department of Characterisation of Materials Structure

Department of Chemical Engineering and Technology

Department of Electrochemical Material Science

Department of Environmental Research

Department of Functional Materials and Electronics

Department of Fundamental Research

Department of Laser Technologies

Department of Molecular Compound Physics

Department of Nanoengineering

Department of Nanotechnology

Department of Nuclear Research

Department of Optoelectronics

Department of Organic Chemistry

Department of Physical Technologies

Department of Textile Technologies

Laboratory of Electronic Processes

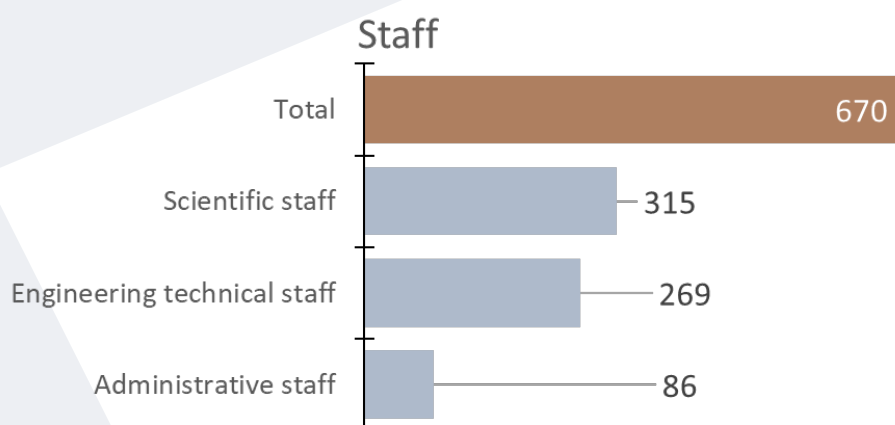


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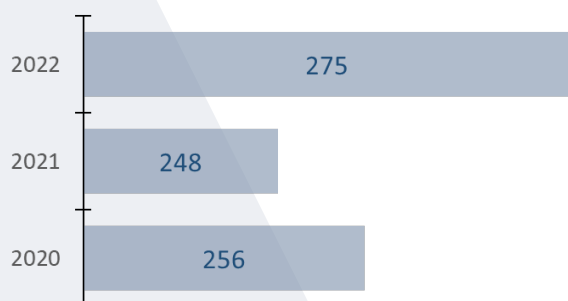
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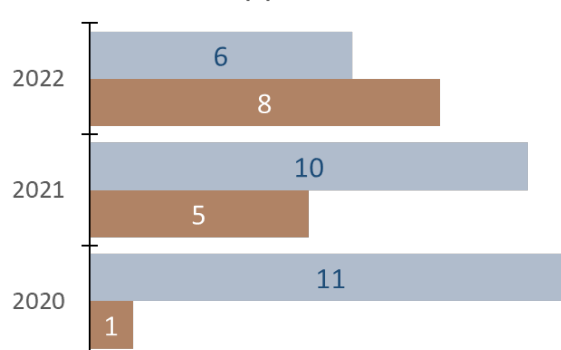
# Facts & figures



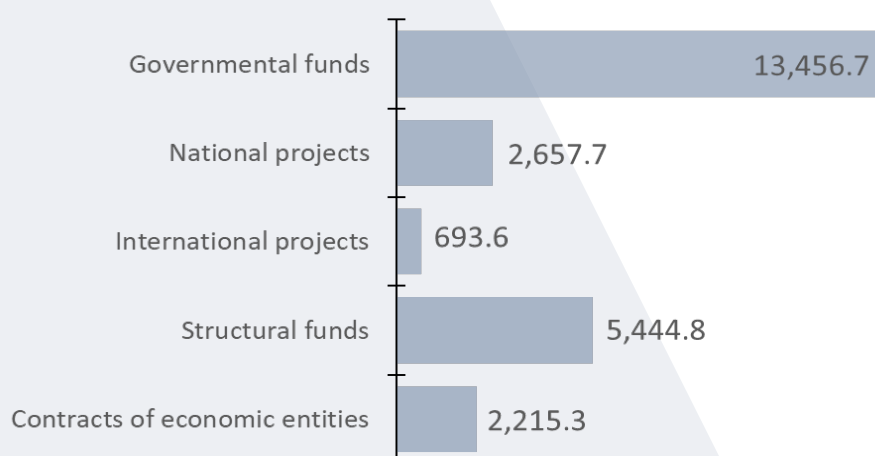
■ Publications



■ Patents  
■ Patent applications



Total budget – 24,468.1 kEur





# Doctoral theses

## SIMONAS RAMANAVIČIUS

Formation, modification and new applications of orderly structured titanium oxide nanostructure. (N 003)

Scientific supervisor: dr. A.Jagminas

## PAULIUS MACKONIS

Development of a high peak power laser based on solid-state, parametric and stimulated Raman amplifiers. (T 008)

Scientific supervisor: dr. A.Rodin

## LAIMA KAZAKEVIČIŪTĖ-JAKUČIŪNIENĖ

Investigation of  $^{137}\text{Cs}$  and Pu isotopes accumulation in soil. (N 003)

Scientific supervisor: dr. E.Maceika

## ADRIÁN VICENT CLARAMUNT

Study on different applications of volatile organic compounds using thermal desorption with gas chromatography. (N 003)

Scientific supervisor: dr. E.Naujalis

## EVELINA DUDUTIENĖ

Photoluminescence properties of GaAsBi quantum wells and Bi quantum dots. (N 002)

Scientific supervisor: prof. dr. G.Valušis

## RAMINTA STAGNIŪNAITĖ

Development of metal oxide-based catalysts and their application for fuel cells (N 003)

Scientific supervisor: dr. V.Kepenienė

## ARNAS NAUJOKAITIS

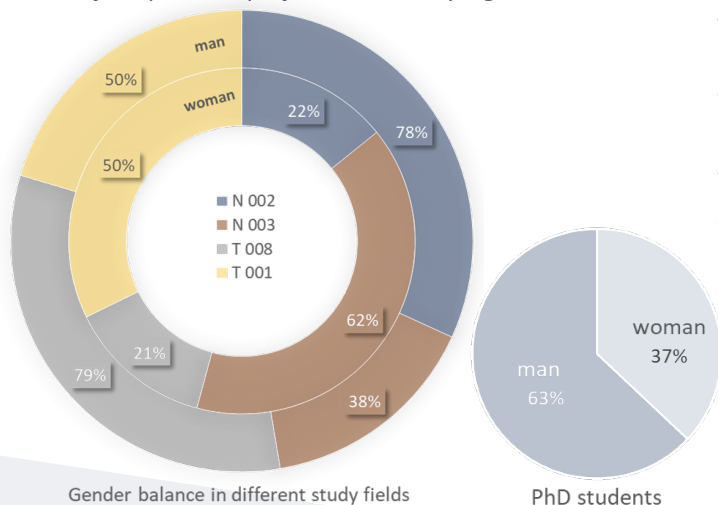
Hydrothermal synthesis of Molybdenum disulfide ( $\text{MoS}_2$ ) heterostructures for the hydrogen evolution from water. (T 008)

Scientific supervisor: dr. A.Jagminas

## AUGUSTINAS POVILAS FEDARAVIČIUS

Algorithms of synchronization control in neural networks. (N 002)

Scientific supervisor: prof., habil. dr. K.Pyragas



25 New PhD students

17 Defended doctoral theses

122 PhD students in total

## ANDRIUS ŽEMAITIS

Efficient laser ablation for bio-inspired 3D functional surfaces. (T 008)

Scientific supervisor: dr. M.Gedvilas

## DARIUS URBONAS

Silicon micro ring resonators decorated by metal and perforations for optical sensors. (T 008)

Scientific supervisor: dr. R.Petruškevičius

## MALIHA PARVIN

Photoelectrochemical synthesis of strong oxidants using tungsten (VI) oxide. (N 003)

Scientific supervisor: dr. J.Juodkazytė

## ERNESTA BUŽAVAITĖ-VERTELINĖ

Strong coupling of hybrid Tamm and surface plasmon polaritons states. (N 002)

Scientific supervisor: dr. Z.Balevičius

## JUOZAS DUDUTIS

Volumetric modification and processing of transparent media by inducing cracks in the material with laser beams of various spatial structure. (N 002)

Scientific supervisor: dr. P.Gečys

## ALGIRDAS PABEDINSKAS

Radiocarbon dispersion in the atmosphere and accumulation in the biosphere analysis in the environment of a nuclear facility. (N 002)

Scientific supervisor: prof., dr. V.Remeikis

## ZITA ŽUKAUSKAITĖ

Application of biosorbents for the determination of Cs and Pu isotopes in freshwater. (N 003)

Scientific supervisor: dr. R.Druteikienė

## RIČARDAS NORKUS

Terahertz pulse excitation spectroscopy of semiconductor materials and structures. (N 002)

Scientific supervisor: prof., habil.dr. A.Krotkus

## AGNĖ ZDANIAUSKIENĖ

Characterization of biomolecules by shell-isolated nanoparticle-enhanced Raman spectroscopy. (N 003)

Scientific supervisor: prof., habil.dr. G.Niaura



# Main projects

European Commission project

**Advancing Science and TEchnology thRough  
dlamond Quantum Sensing – ASTERIQS**

**A. Alkauskas**

European Commission project

**In-built Triggered Enzymes to Recycle Multi-layers:  
an Inova-tion for Uses in Plastic-packaging –  
TERMINUS**

**S. Asadauskas**

European Commission project

**European Joint Research Programme  
in the management and disposal of radioactive  
waste – EURAD**

**R. Plukienė**

Horizon 2020 programme project

**PRE-DISposal management of radioactive  
waste – PRE-DIS**

**R. Plukienė**

Horizon 2020 programme project

**Fostering the PAN-European infrastructure for  
empowering SMEs digital competences  
in laser-based advanced and additive  
manufacturing – PULSATE**

**G. Račiukaitis**

Horizon 2020 programme project

**Laser-plasma based source 3D Tomography  
for cargo inspection – MULTISCAN 3D**

**G. Račiukaitis**

Horizon 2020 programme project

**Innovation fostering in accelerator science and  
technology**

**V. Tomkus**

ResearchExecutive Agency (REA) project

**Chalcopyrite-perovskites for infrared  
photovoltaics – IRPV**

**R. Kondrotas**

Research Executive Agency (REA) project

**Dirac Semimetals based Terahertz Components –  
DiSeTCom**

**G. Valušis**

Research Executive Agency (REA) project

**Terahertz Photonics for Communications,  
Space, Security, Radio-Astronomy, and  
Material Science – TERAOPTICS**

**I. Kašalynas**

Research Executive Agency (REA) project

**FLuorescent nanO-agents for super-Resolution  
Imaging and seNsing – FLORIN**

**R. Karpič**

European Space Agency (ESA) project

**Bismide-based Intersubband Devices  
for Mid-Infrared Applications – BISMIRA**

**J. Devenson**

European Space Agency (ESA) project

**Optical fiber-based source of entangled  
photons for satellite-based quantum  
communications – EPhOS**

**V. Tomkus**

Science for Peace and Security Programme project

**Tuned optical sensors for detection and  
identification of airborne hostile agents –  
HOSTITUNOP**

**A. Rodin**

European Health and Digital Executive Agency project

**Evidence Driven Indoor Air Quality  
Improvement – EDIAQI**

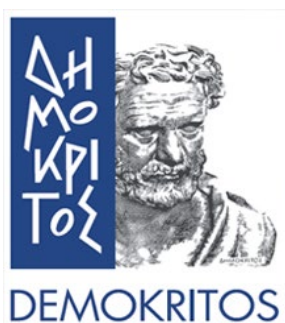
**S. Byčenkienė**

European Defence Fund project

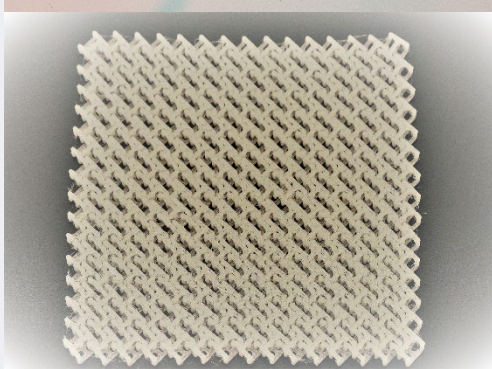
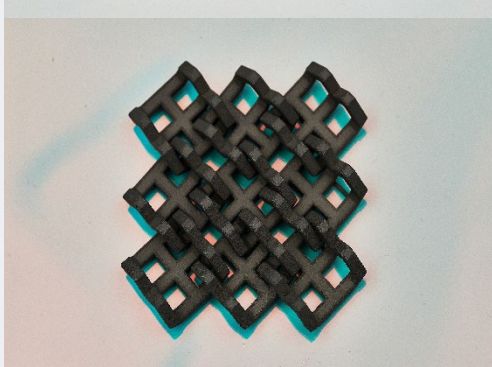
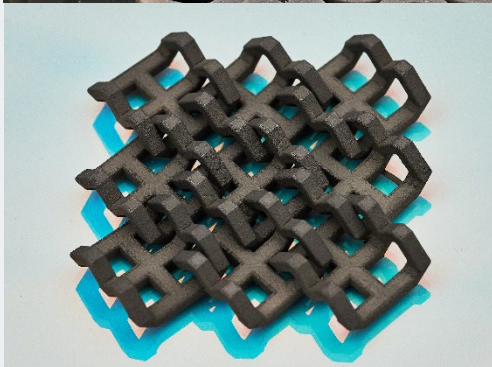
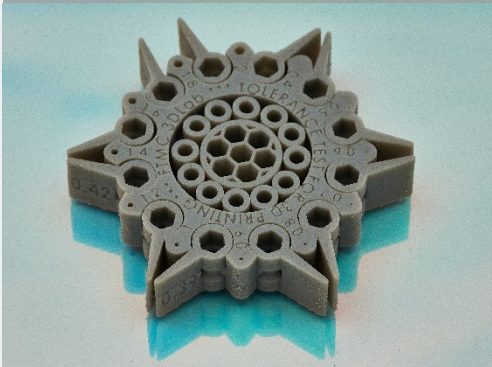
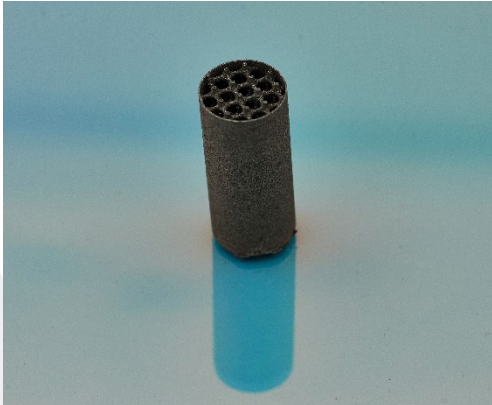
**Additive Manufacturing of Lightweight  
Laser Target Designator – AMLTD**

**G. Mordas**

# Projects partners







# Patents

## Method for fabrication of recessed electrical elements



EP3975224B1

2022.11.30

Irmantas Kasalynas, Simonas Indrisiunas, Pawel Prystawko, Piotr Kruszewski

The invention relates to the technical field of microelectronic components and is related to the forming of recessed and regrown electrical contacts for wide-bandgap group III nitride semiconductor components. In the regions of the heterostructure, intended for the forming of the recessed elements, each recess is formed using laser micro-processing. The top surface of the heterostructure of the III-N semiconductor layer, grown on the substrate, is coated with at least one protective layer in order to form a blank. The blank is placed in a chamber, vacuumed or filled with an inert or shielding gas, and the recess are formed separately for each contact and/or junction and/or electrical component. For this, the focused ultrashort pulsed laser radiation is directed through the transparent window in the chamber and used to remove the protective layer and required thickness of the material of the heterostructure layers, forming the recess with required depth in the said heterostructure. The blank and focused laser beams are translated with respect to each other in the controlled manner to form the next recess in the same way.

## Method of polymethylmethacrylate (PMMA) removal from graphene surface by photoexposure



LT6888B

2022.01.25

Natalia Alexeeva, Irmantas Kasalynas

Method relates to the technical field of material science. The method of removal comprises following steps: PMMA, used as a supportive or mask layer for graphene on a substrate (PMMA/graphene/substrate), is subjected to DUV to expose PMMA using its photosensitive properties; exposed PMMA is developed in alcohol/water mixture releasing the surface of graphene. Graphene/substrate is dried by nitrogen.

## Low contact resistance device and method of production



EP3840050B1

2022.03.09

Steponas Asmontas, Jonas Gradauskas, Konstantinas Leinartas, Laurynas Stasiunas, Algirdas Suziedelis, Aldis Silenas

The invention relates to the field of electronics associated with the design and manufacture of semiconductor devices which require low contact resistance between titanium dioxide (TiO<sub>2</sub>) and p-type conductivity semiconductor. The proposed device is a layered structure comprised of a heavily doped p-type semiconductor layer and a n-type TiO<sub>2</sub> layer arranged thereon, and a tunnel junction is formed between these layers. In order to reduce the number of technological operations, the time and materials used to form a low resistivity contact, the TiO<sub>2</sub> layer is directly deposited on the p-type semiconductor by atomic layer deposition (ALD) method, while the part of the TiO<sub>2</sub> layer adjacent to the p-type semiconductor surface is additionally doped with niobium (Nb) donor impurity during the ALD-growth process, thus forming a tunnel junction between the TiO<sub>2</sub> n-type layer and the p-type semiconductor.

## Manufacturing method for recessed electrical components



LT6909B

2022.04.25

Irmantas Kasalynas, Simonas Indrisiunas,  
Pawel Prystawko, Piotr Kruszewski

The invention relates to the technical field of microelectronic components and is related to the forming of recessed and regrown electrical contacts for wide-bandgap group III nitride semiconductor components. In the regions of the heterostructure, intended for the forming of the recessed elements, recess are formed using laser micro-processing. The top surface of the heterostructure of III-N semiconductor layer, grown on the substrate, is coated with at least one protective layer in order to form a blank. The blank is placed in a chamber, vacuumed or filled with an inert or shielding gas and the recess are formed separately for each contact and/or junction and/or electrical component. For this, the focused ultrashort pulsed laser radiation is directed through the transparent window in the chamber and used to remove the protective layer and required thickness of the material of the heterostructure layers, forming the recess with required depth in the heterostructure. The blank and focused laser beams are translated with respect to each other in the controlled manner to form the next recess in the same way. The formed recess is filled with either the doped III-N semiconductor layer and/or metal compounds, forming the recessed electrically conductive contact and/or electrically partially conductive contact and/or junction and/or electrical component.

## Method for electroless nickel deposition onto copper without activation with palladium



LT6899B

2022.04.11

Aldona Jagminiene, Ina Stankeviciene, Karolis Ratautas,  
Eugenijus Norkus, Gediminas Raciukaitis

The invention relates to selective deposition of a nickel layer on a copper surface. The invention may be used in the production of electrically conductive areas for electronic circuits. Method for nickel deposition on the surface of copper comprises immersing an item, which surface is to be deposited with the nickel layer, into one or more baths, of which at least one contains a reducing agent and of which at least one is adapted for (electroless) plating of nickel. In order to extend the field of application and to obtain practically pure nickel coatings, said reducing agent comprises boronic or phosphoric compounds, comprising morpholine borane ( $C_4H_9BNO$ ), or dimethylamine borane ( $C_2H_7BN$ ), or sodium tetrahydroborate ( $NaBH_4$ ), or sodium hypophosphite ( $NaH_2PO_2$ ) and said reducing agent directly or indirectly reduces insoluble copper(I) or copper(II) compounds on the copper surface. At least one of the mentioned baths comprises a ligand or mixture.

## Tandem two-terminal perovskite-silicon multilayer solar cell

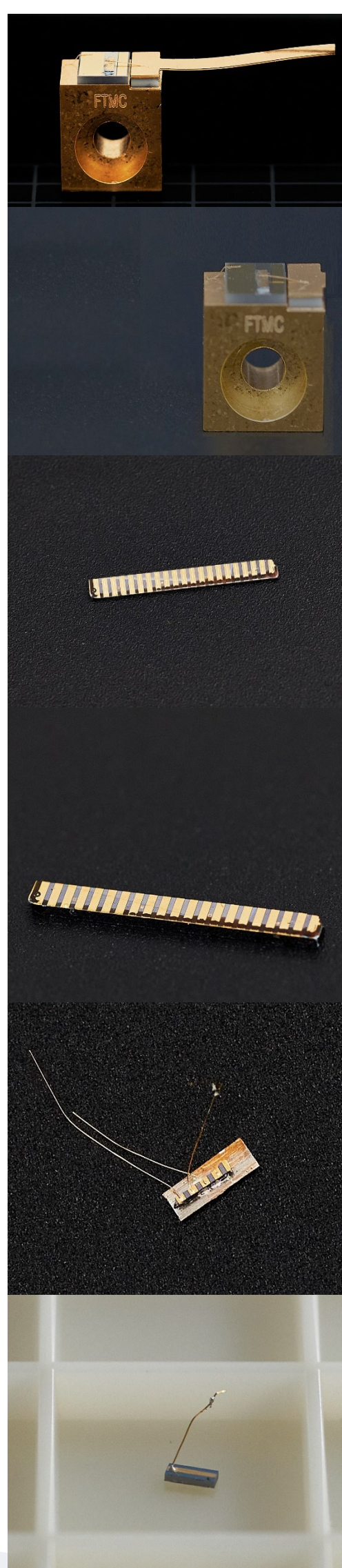


LT6970B

2022.12.27

Steponas Asmontas, Jonas Gradauskas, Asta Griguceviene,  
Konstantinas Leinartas, Kazimieras Petrauskas, Laurynas Staisiunas,  
Algirdas Suziedelis, Aldis Silenas, Edmundas Sirmulis

The invention relates to the field of solar cells. The proposed tandem solar cell consists of two solar cells, perovskite and crystalline silicon, connected in series, and their good contact is provided by a semiconductor tunnel junction featuring low electrical and optical losses. The advantage of the proposed perovskite/silicon solar cell is achieved by the fact that it does not require fabrication of the tunnel junction as a separate additional structure, but the tunnel junction is formed by appropriate doping of electron transfer layer of the perovskite cell during the fabrication of the layer. Thus, production of the tandem perovskite/silicon solar cell involves fewer technological operations and requires less materials, and the tunnel junction being above the silicon solar cell demonstrates low ohmic resistance within the low-voltage range and does not absorb light photons required to generate electrons and holes in the silicon solar cell.



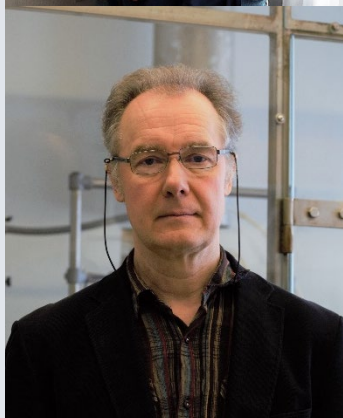


# Awards



## Lina Grinevičiūtė

For breakthrough in optical coatings technologies and the best PhD thesis in Lithuania in 2022.



## Linas Labanauskas

For long standing activities and permanent innovation in organic materials synthesis, for a number of international R&D projects with high-tech industry.



## Evaldas Tornau

For contribution in developing of theoretical models and numerical engineering of molecular assemblies and phase transitions in advanced materials; for his more than a decade dedication to Lithuanian Journal of Physics.



## Milda Tamošiūnaitė-Survilienė

For accurate and remarkable work in managing reports and information related to the Sunrise Valley project dedicated to establish National Centre for Physical Sciences and Technology, for FTMC organized conferences and innovation activities within the last decade.



## Albertas Malinauskas

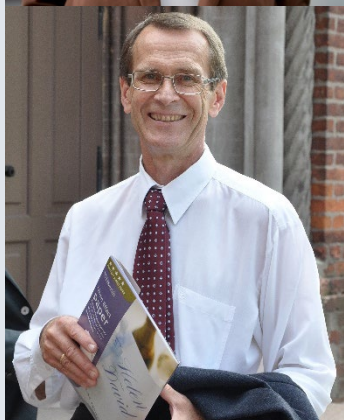
For life achievements: for groundbreaking innovations in electro-chemistry of organic compounds; for providing strength, scientific direction and values, unifying and mobilizing, motivating and igniting; for all that has already been and will be created.

# Special awards



## Ieva Plikusienė for talent perspective

For encouraging results and promising projects, for extending scientific activities within the country and abroad.



## Vytautas Karpus for classical courses for PhDs

For top level courses in Solid State Physics and Quantum Semiconductor Structures given for PhD students of the Center. For the standard in scientific precision and teaching, for patience and tolerance, for inexhaustible sharing of knowledge and scientific experience

# FTMC patronage award



## Marius Jakulis Jason Founder of Marius Jakulis Jason Foundation

For Good Will in financial support of talented academics eager to contribute to scientific and technological growth of Lithuania.



# Events



## Lithuanian-Taiwan Semiconductor and Materials Science Center starts its activities at FTMC

On February 17, the joint Taiwan and Lithuania Center for Semiconductors and Materials Science was opened at FTMC. On this occasion, the founders of this new research and innovation development center, FTMC and National Taiwan Sun Yat-Sen University, held a live online conference for researchers. /2022.02.18/



## FTMC scientist wins the international competition Dance Your PhD

Dr. Povilas Šimonis participated in the international competition Dance Your PhD and became the overall and biology category winner. He created a video depicting the "dance" of yeast cells and presented his research in this original way. Yeast is a single-celled fungus that powers baking and hosts other biological processes. In his research, carried out at FTMC, P. Šimonis studied the response of yeast cells to a pulsed electric field. Exposure

to a pulsed electric field can increase the permeability of various cell membranes, deactivate them, or make them more efficient. Such research is important for the application of electroporation in the food industry and biotechnology. What is the recipe for a playful award-winning video? Basically the same as a good pastry - you need to plan, use good quality ingredients and have the patience to wait for the yeast to do the main job. /2022.02.24/



## Directors of Lithuanian State Research Institutes express support for Ukraine

As Russia waged widespread military aggression against Ukraine, the Conference of Directors of Lithuanian State Research Institutes unanimously expressed its solidarity with the independent state of Ukraine and its people, who are fighting today for the freedom of all of us. Aggressor troops are attacking Ukrainian cities; civilians, homes, kindergartens, schools and universities are being shelled. These actions are totally unacceptable in the 21st century and put the whole world at risk. On behalf of all 11 Lithuanian research institutes, the Directors condemned the violence and aggression that puts thousands of our colleagues across Ukraine at risk and expressed our support and encouragement to all the Ukrainian people and research community.

Also, #ScienceForUkraine platform has been launched, which announces various opportunities for Ukrainian scientists and students. PhD students and researchers are being welcomed to FTMC to study and work in the fields of laser technologies, optoelectronics, nuclear physics, organic chemistry, bio- and nanotechnologies, electrochemical material science, functional materials, electronics, etc. /2022.03.01/



## 65th international conference Open Readings 2022

The 65th international conference for students of Physics and Natural sciences Open Readings 2022 took place in FTMC on 15-18 of March, 2022.



## International relations of FTMC are strengthening

On March 17, FTMC was visited by the Ambassador Extraordinary and Plenipotentiary of Japan to Lithuania Tetsu Ozaki and the First Secretary of the Japanese Embassy Hiroshi Okasaki. The purpose of the visit was to strengthen mutual scientific cooperation between Japan and Lithuania. /2022.03.17/

A delegation of scientists, businessmen, and officials from Taiwan's advanced semiconductor technology institutions also visited the FTMC in March. During the visit, the guests from Taiwan took part in a seminar, where they presented the scientific research centers and academic institutions they represent (ITRI, NarLabs, etc.), ongoing research and developing technologies, possible cooperation and investment prospects. **/2022.03.23/**



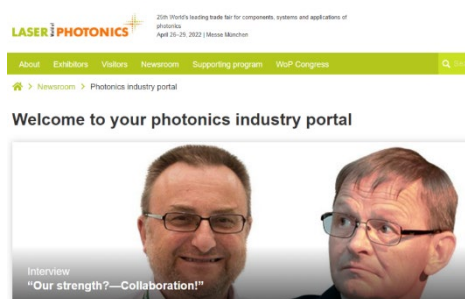
Vice Minister of Foreign Affairs of Poland Paweł Jabłoński visited FTMC and high-tech company "Ekspla". The Vice Minister was acknowledged with the activities of FTMC in the field

of photonics and the cooperation between FTMC and Polish scientific institutions. During the meeting, the development of cooperation between Poland and Lithuania was discussed. **/2022.04.08/**

On May 9, FTMC Director Gintaras Valušis and the president of the Korean Institute of Machinery and Materials Science (KIMM) Park Sang-Jin signed a Memorandum of Understanding (MoU) and Cooperation between the two scientific institutions. The memorandum aims to strengthen the cooperation between FTMC, the leader in research and innovation development in the Baltic states, and KIMM, the state institute of applied sciences in South Korea, in the fields of laser optics, ultrashort pulse lasers and laser micromachining. **/2022.05.09/**



Head of the Department of Laser Technologies at FTMC dr. Gediminas Račiukaitis has been elected vice-chairman of the Extreme Light Infrastructure/European Research Infrastructure Consortium (ELI ERIC). **/2022.03.24/**

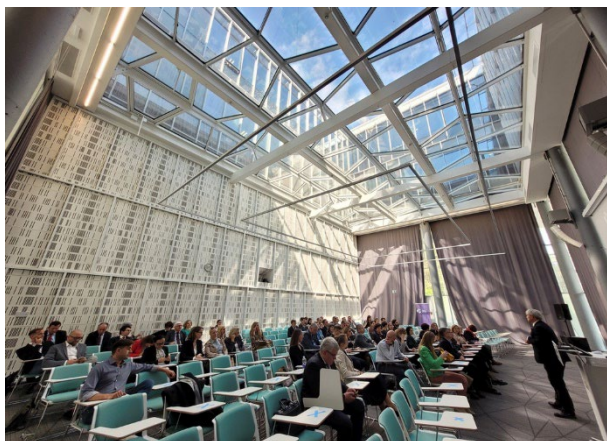


## Gediminas Račiukaitis gave an interview for Photonics Industry Portal

A highly dynamic photonics industry is forming in Lithuania. Gediminas Račiukaitis, President of the Lithuanian Laser Association and Head of the Laser Technologies Department at FTMC, has accompanied the rise of the strongly exports-oriented industry from the very beginning. Among its pioneers is also Kestutis Jasiūnas, CEO of EKSPLA, a laser manufacturer founded in 1992. Its ultrafast lasers are used in top research facilities around the globe.



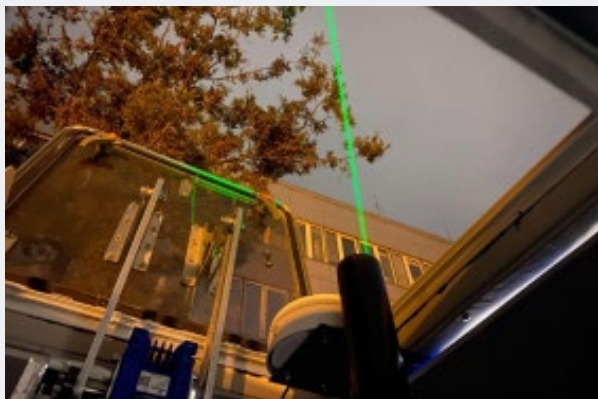
In their interview, Jasiūnas and Račiukaitis talk about the scientific roots of their industry, the increasing diversity of solution providers across the entire process chain, and about joint trade fair booths as a lever to promote Lithuania as an innovative photonics hub. **/2022.04.21/**



## Visit of a delegation of Lithuanian economic diplomats

A large delegation of diplomats and special attachés responsible for Lithuanian and foreign economic relations and their development visited FTMC. The meeting was attended by more than sixty representatives of Lithuania responsible for the economic interests of our country in diplomatic missions around the world. **/2022.05.30/**

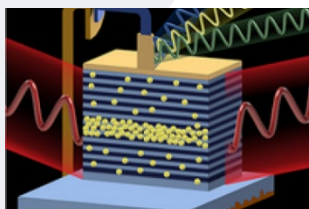




### **LIDAR measurements – unique Lithuanian and Polish scientific project: for the first time remote sensing study on aerosol properties modifications will be conducted between observational sites**

Aerosol pollution, one of the main factors destabilizing Earth's climate, kills 6-9 million people each year. World environmental and climate change experts confirm that reducing released carbon emissions is the important part of combatting climate change. But recently it was mistakenly declared that biomass burning is a carbon-neutral source of energy. As scientists emphasize, in reality the burning of biomass emits wide ranges of aerosol particles and gases

into the atmosphere, which significantly affects regional air quality, global atmospheric chemistry, biogeochemical cycles and Earth's radiative budget. FTMC together with University of Warsaw, Faculty of Physics started the project Importance of long-range transport of BIO mass burning emissions to local Smog events in Urban Environments (BIOSURE). This unique two-years international investigation is going to provide an unique possibility separately to evaluate the importance of local and long-range transport of biomass burning-related aerosol to the air quality in urban environments. /2022.06.07/



### **The prestigious journal Physical Review Letters recommended the publication of FTMC scientists**

Physical Review Letters, with a tag 'recommended by editors', published an article of international group of scientists from FTMC, Poland, Finland, Germany and the UK, V. Čižas, L. Subačius, N. V. Alexeeva, D. Seliuta, T. Hyart, K. Köhler, K. N. Alekseev and G. Valušis, entitled "Dissipative Parametric Gain in a GaAs/AlGaAs Superlattice". The main goal of the paper was to show the long-awaited experimental proof of



parametric amplification in quantum superlattices. /2022.06.14/



### **International Electroanalysis Conference ESEAC 2020/2022**

The 18th International Electroanalysis Conference ESEAC 2020, postponed twice due to the COVID-19 pandemic, finally took place in Vilnius in June. The international event was organized by FTMC and the Life Sciences Center of Vilnius University. Chairwoman of Scientific and Organizational Committees was prof. Rasa Pauliukaitė from FTMC. /2022.06.27/



### **Albertas Malinauskas honoured with a Lithuanian State Award**

On July 6, the Day of the State of Lithuania, the Coronation of King Mindaugas and the National anthem, the President of the Republic of Lithuania, Gitanas Nausėda, awarded the Knight's Cross of the Order of the Grand Duke Gediminas to prof. Albertas Malinauskas, the head of the Department of organic chemistry of FTMC, the author of research in organic chemistry and inventions applied to medicine, food industry and environmental research. /2022.07.06/



### **The Prime Minister of Luxembourg visited FTMC**

On September 5, the Prime Minister of the Grand Duchy of Luxembourg Xavier Bettel, who arrived in Lithuania for a several-day visit, together with the Lithuanian Minister of Economy and Innovation Aušrinė Armonaitė and a delegation of diplomats visited FTMC. Director of the center Gintaras Valušis briefed the guests on the activities and competences of FTMC in the fields of lasers, other high-tech innovations, and space technologies. /2022.09.05/

## The technology of FTMC scientists is conquering the photonic industries

A fundamental solution developed and patented by one of the founders of Litilit company together with FTMC enables the production of ultra-short optical pulse lasers up to 100 times more efficient than it was possible before. The first 1.6 million euros investment attracted when it was just a team of four experts, now the start-up is planning for expansion. The short-term plan is 50 people producing one laser (costing about 100 thousand euros) per day. The long-term plan is a unicorn start-up and a new market standard with advanced processes available to everyone. The extremely short light pulse generator developed by the Lithuanian start-up is already used in the semiconductor and electronics industry, medical equipment, processing and production of various materials, eye surgery, microscopy, even space research. /2022.09.06/



### Leaders of optoelectronics and photonics gather at FTMC: international conference APROPOS 18

On October 2-7, FTMC, the leader in innovation and scientific research in Baltic countries, invited prominent scientists in photonics to the international scientific conference APROPOS 18. The conference Advanced Properties and Developments in Optoelectronic Materials and Systems (APROPOS), which has a more than half a century tradition being held in Vilnius, was organized for the 18th time. Since first symposium Plasma and instabilities in semiconductors in 1971, the APROPOS conference eventually became a forum focused mainly on topics of optoelectronics and semiconductor devices and terahertz technology. It reflects current and scientific breakthrough trends in optoelectronic materials and technologies, semiconductor physics and photonics. /2022.10.02-07/



The week of events of APROPOS 18 started with the master class of the TERAOPTICS project for PhD students working in the field of terahertz optics. During the training, the participants were very fond of the interactive format, to opportunities to express themselves, but not just to listen to the training material. Twenty seven highly motivated participants from various European countries participated in the course. /2022.10.02-03/



### The visit of Belgian King Philippe to FTMC boosting bilateral cooperation

In October, the Belgian royal couple, King Philippe and Queen Mathilde, came to Lithuania for the official state visit and paid a visit to biotechnology research institutions in Vilnius Saulėtekis Valley. During the visit to FTMC, the director of the center Gintaras Valušis presented the activities and competences of FTMC in the fields of scientific research and high technology development. Later, a short excursion was arranged, and the guests visited the Spectrometry Laboratory of Nuclear Research Department, Optoelectronics Department and Optical Coherence Tomography

Laboratory, where the chief scientists of these units, V. Remeikis, L. Minkevičius and E. Aukorius, introduced the activities of their units. The King of Belgium Philippe and Queen Mathilde took a special interest in the research of FTMC Spectrometry Laboratory and the objects prepared for scientific investigation there. The visit to FTMC and other scientific institutions was a part of a state visit to honor the century-long bilateral relations and solidarity between Lithuania and Belgium. /2022.10.28/





### Karolina Maleckaitė, PhD student at FTMC, triumphed in the first science popularization competition Researchers Grand Prix

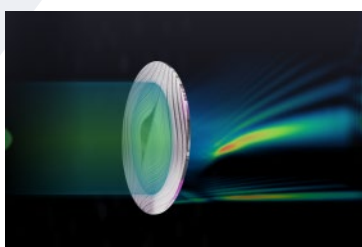
She explained why she is interested in studies of cell viscosity and why this research is relevant to society. According to Karolina, one of the reasons why she decided to participate in the competition was to challenge herself and learn to present complex scientific subjects in a simple way. 10/27/2022



### Designer Serge Gandzumian and the scientists of Department of Textile Technology created a collection of clothes made of self-degrading fabrics

The researchers of the Department of textile technology of FTMC with their partners - designer Seržas Gandžumianas company MB Grata forma

and consulting and IT solutions company UAB PPM Consulting, completed the project Eco-design leisure clothing from natural and biodegradable fibers, based on circular economy principles of the international EUREKA program coordinated by MITA. The project aims to introduce sustainable eco-design products to the global fashion market using biodegradable fibers. The project promoters created innovative, self-degrading and/or recyclable textile materials and their products. Fashion designer S. Gandzumian created a collection of leisure clothes from the woven and knitted materials from biodegradable hemp, polylactide, lyocell, wool fibers and their mixtures produced by FTMC researchers. /2022. 10. 28/



### Publication by FTMC researchers in the Nature group journal Light: Science & Applications

In November, one of the world most influential optical journals, Light: Science & Applications (a member of the Nature group) published a joint research of scientists from the Optoelectronics and Fundamental Research Departments of FTMC, R. Ivaškevičiūtė-Povilauskienė, P. Kizevičius, E. Nacius, D. Jokubauskis, K. Ikamas, A. Lisauskas, N. Alexeeva, I. Matulaitienė, V. Jukna, S Orlov, L. Minkevičius, G.

Valušis, Terahertz structured light: nonparaxial Airy imaging using silicon diffractive optics. The article is devoted to the generation of terahertz structured light using planar photonic cells and its application for imaging of objects and two-dimensional materials. /2022. 11. 22/



### Young scientist L. Grinevičiūtė from FTMC became the winner of the best thesis competition

On November 22, the President of the Republic of Lithuania Gitanas Nausėda awarded the authors of the best scientific dissertations of 2021. The best dissertation in natural, technological, medical and health, and agricultural sciences was defended by Lina Grinevičiūtė on the topic Nanostructured optical coatings for laser light control (FTMC, scientific supervisor Ramutis Drazdys). /2022. 11. 22/



### FTMC researcher Ieva Plikusienė - Lithuanian woman of the year

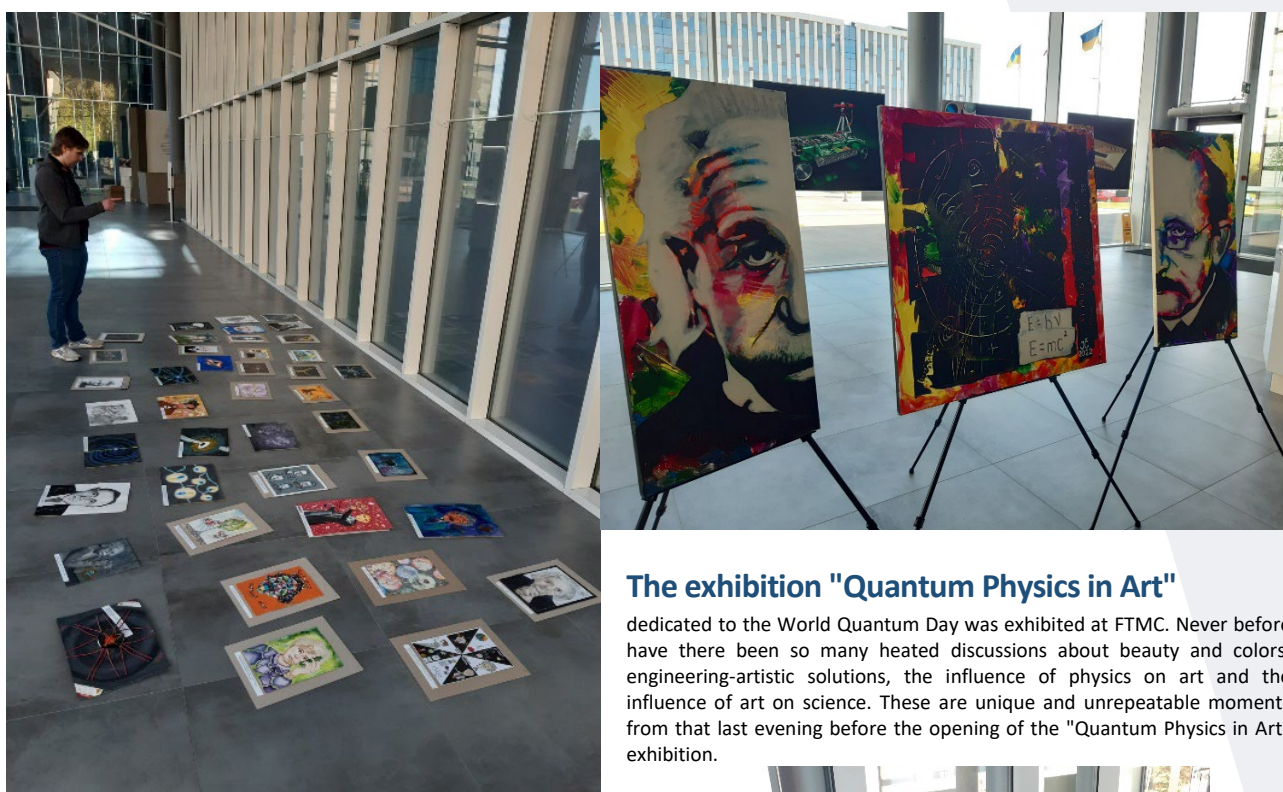
In December, the 2022 Lithuanian Woman of the Year, according to Lietuvos rytas Stilius edition, was announced - this year this honorable title went to Ieva Plikusienė, a scientist from FTMC and a lecturer of Vilnius University, Faculty of Chemistry and Geosciences. The work of Plikusienė, who has been researching biological sensors for 13 years, became particularly significant after the onset of the coronavirus. The research she and her team was conducting helps to obtain important information needed to create more accurate rapid tests, as well as to characterize antibodies used for treatment. /2022. 12. 08/



## A book on quantum computing has been published in Lithuania

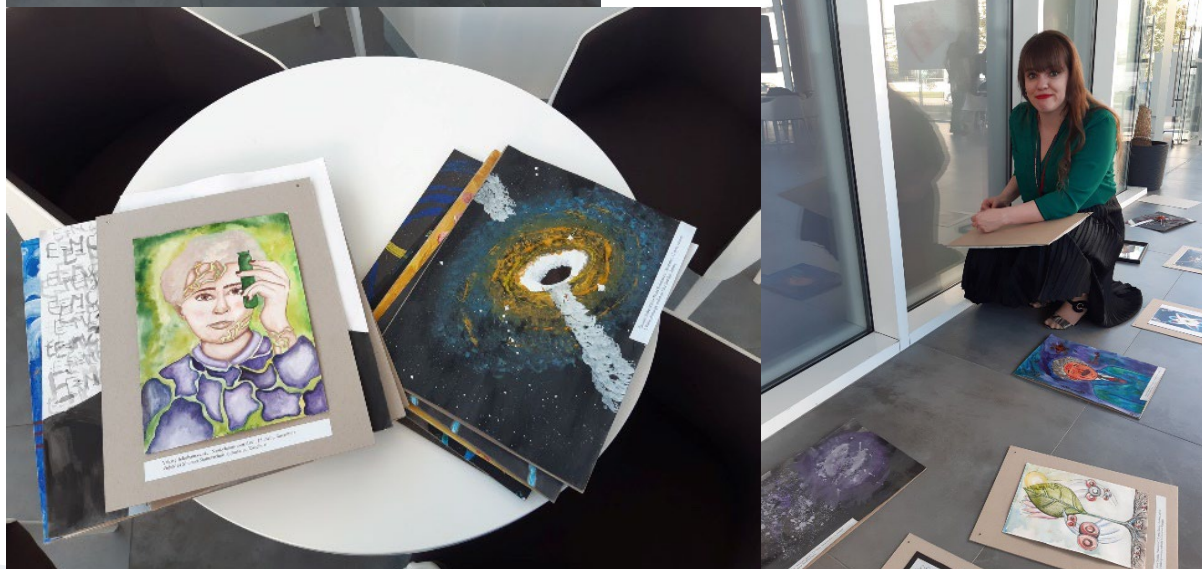
Physicists Tadas Paulauskas (FTMC, Optoelectronics Department, Laboratory of Optoelectronics Technologies) and Julius Ruseckas (Baltic Institute of Advanced Technologies) published a book Quantum computing in Lithuanian. The book is openly available on the internet at: [www.kvantinekomputerija.lt](http://www.kvantinekomputerija.lt). The book covers main introductory topics, from the operation of quantum logic gates, fundamental algorithms, quantum communication protocols to the principles of quantum error correction. /2022. 12. 08/

# Beyond science



## The exhibition "Quantum Physics in Art"

dedicated to the World Quantum Day was exhibited at FTMC. Never before have there been so many heated discussions about beauty and colors, engineering-artistic solutions, the influence of physics on art and the influence of art on science. These are unique and unrepeatable moments from that last evening before the opening of the "Quantum Physics in Art" exhibition.

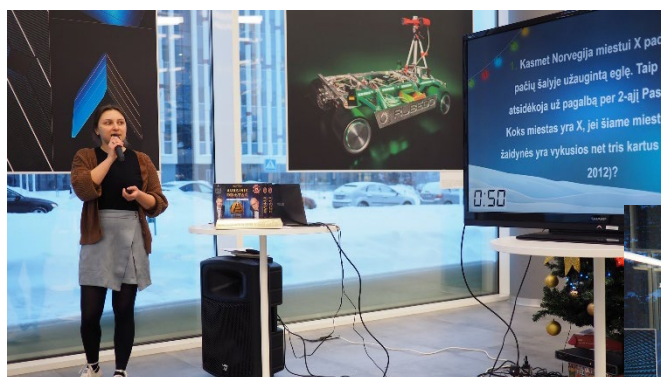






### FTMC PhD students Lena Golubewa, Yaraslau Padrez and Raman Novikau

participated and won prizes in the marathons *We run Vilnius*, *Vilnius Rimi Marathon*, *Širvintai Marathon* and also in *Warsaw Half Marathon* held in Poland.



**The FTMC Christmas mindfight quiz attracted a lot of interest** – as many as fifteen teams competed with each other. There was an intense point-to-point battle for the best places and great prizes.

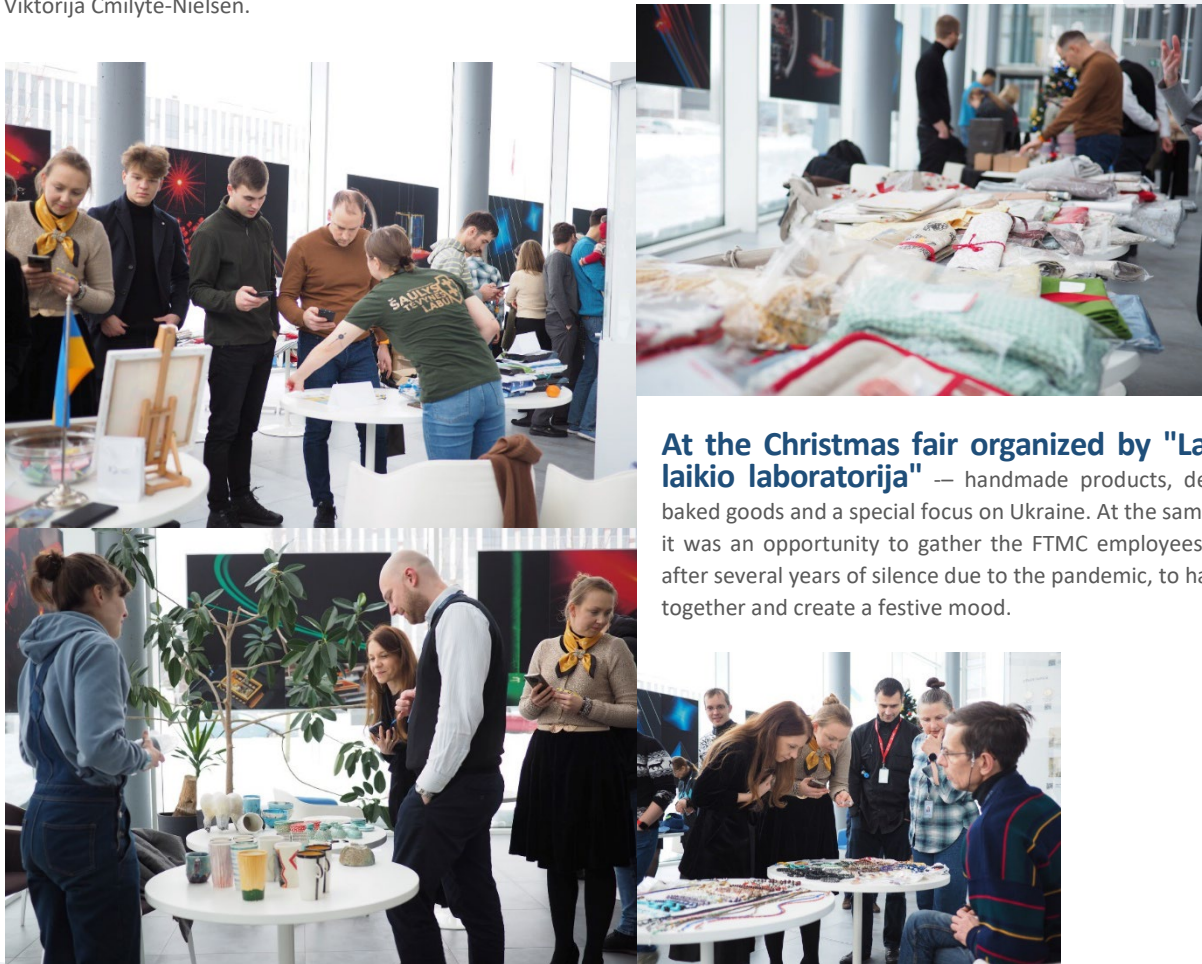






### The 3rd FTMC Chess Tournament

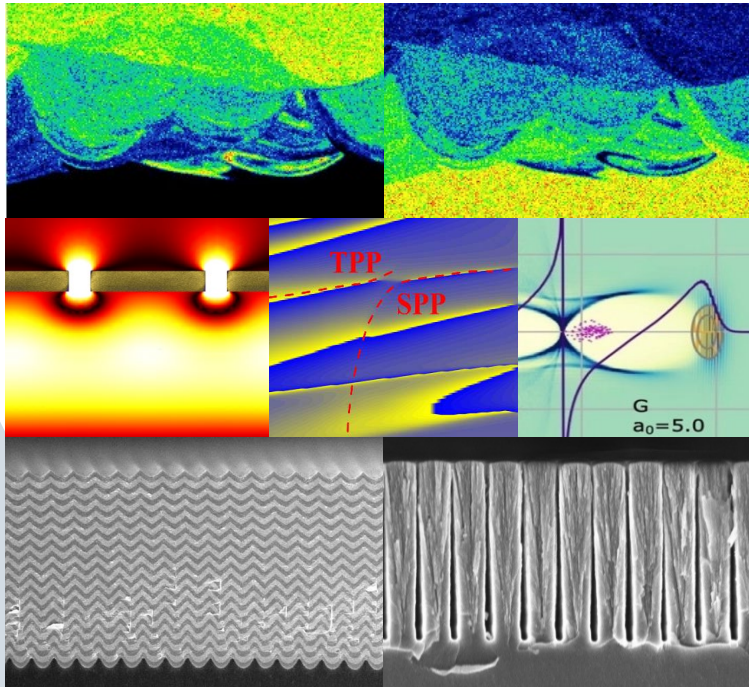
was organized to popularize among our scientific community the sport of chess, a game symbolizing intelligence, diligence, insight, courage and wisdom. The winners of the tournament earned the opportunity to compete with chess grandmaster Viktorija Čmilytė-Nielsen.



**At the Christmas fair organized by "Laisvalaikio laboratorija"** — handmade products, delicious baked goods and a special focus on Ukraine. At the same time, it was an opportunity to gather the FTMC employees again, after several years of silence due to the pandemic, to have fun together and create a festive mood.



# Laser technologies



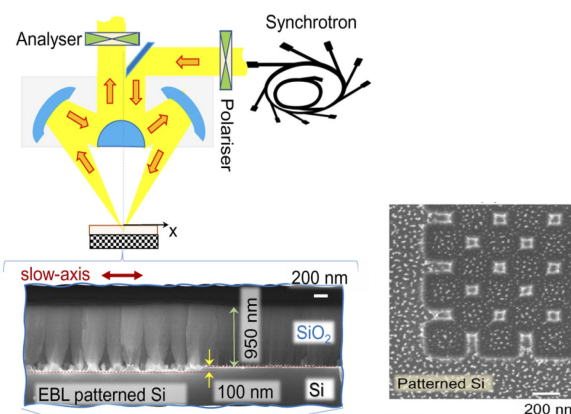
## Along the value chain - optical coatings, solid-state and fibre lasers, plasmonics and nanophotonics, laser material processing and additive manufacturing

The Department of Laser Technologies, with its six laboratories, covers a significant part of the value chain in photonics. New technologies for optical coatings are under development in the Laboratory of Optical Coatings. A piece of glass is transformed into smart optical elements, able to control the spectral, temporal and spatial properties of light. Research at the Fiber Laser and Solid-State Laser Laboratories leads to new principles for generating ultrashort laser pulses and new wavelengths of coherent radiation. Efficient surface texturing utilises laser beam interference for metasurface formation exhibiting plasmonic effects. Glass processing and 3D milling using smart pulsed lasers and shaped Bessel beams, 3D metal sculpturing by subtractive technologies, laser-induced transformations in graphene-like materials and laser structuring for optoelectronic devices make up the primary working topics of the Laboratories of Laser Microfabrication Technologies. The scope of the material processing using ultrashort pulse lasers includes the investigations of the laser-matter interaction and hardware development in the Laboratory of 3D Technologies and Robotics. Significant progress was made in validating novel processes for the electroless plating of laser-modified polymers and glasses. Interaction of ultra-intensive laser beam with gas target leading to Laser Wake Field Acceleration is simulated and experimentally validated with collaborators at leading European laser facilities. The Department collaborates closely with colleagues from other departments of FTMC, and photonics companies in Lithuania and abroad, gaining new ideas for joint projects and applications. The year 2022 was highly fruitful for the Department of Laser Technologies, with new projects and scientific publications in high-ranked peer-review journals.

## Optical anisotropy of glancing angle deposited thin films on nano-patterned substrates

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3D columnar micro-films/coatings were deposited over pre-patterned surfaces with sub-micrometre periodic patterns. Four-angle polarisation analysis of thin ( $0.4 - 1 \mu\text{m}$ ) Si and SiO<sub>2</sub> films, evaporated via glancing angle deposition (GLAD) at  $70^\circ$  to the normal, was carried out in the reflection mode using synchrotron infrared micro-spectroscopy at the Australian Synchrotron. The angular dependence of absorbance followed  $A(\theta) \propto \cos^2\theta$ , confirmed for Si substrates patterned by electron beam lithography and plasma etching, which were used to make checkerboard patterns of  $\Lambda=0.4 \mu\text{m}$  period on a Si substrate. Retardance control by birefringence of a patterned SiO<sub>2</sub> substrate coated by columnar SiO<sub>2</sub> is promising for UV-visible applications due to the use of the same material to endow polarisation control (Fig. 1).

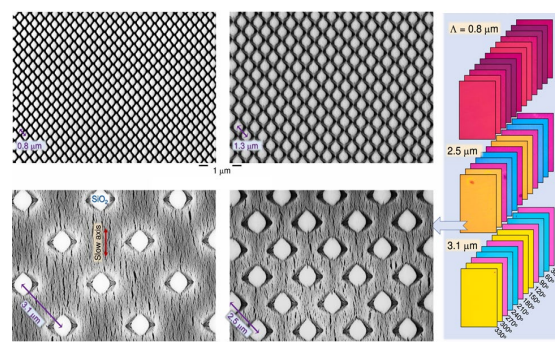


**Fig. 1.** Polariser-Analyser setup used in a reflection mode. (Bottom left) Sample's cross-section along the slow axis; (bottom right) top-view SEM image of a patterned substrate.

## Anisotropic 3D columnar micro-film coating for applications in infrared and visible spectral ranges

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Polarisation analysis of thin ( $\sim 1 \mu\text{m}$ ) SiO<sub>2</sub> films, deposited via evaporation at a glancing angle of  $70^\circ$  to the normal on resist pillar arrays, was carried out using synchrotron-based Fourier transform infrared (s-FTIR) micro-spectroscopy in reflection mode. Changes in the intensity of absorption bands were observed to follow the angular dependence of  $\sim \cos^2\theta$ , consistent with the absorption anisotropy. The strongest absorption was the sharp Si-O-Si stretching vibrational mode at  $1040 \pm 20 \text{ cm}^{-1}$ , which can be used for sensor applications and radiative cooling in the atmospheric transparency window within the range of  $8-13 \mu\text{m}$  ( $1250-769 \text{ cm}^{-1}$ ). Anisotropy of the IR absorbance is correlated with retardance/birefringence of the same patterns in the visible spectral range. Larger period patterns of 3D columnar SiO<sub>2</sub> films of  $\sim 1 \mu\text{m}$  in thickness deposited on polymer/resist pillar arrays provide the possibility to control anisotropy of the form-birefringent 3D columnar films (Fig. 2).

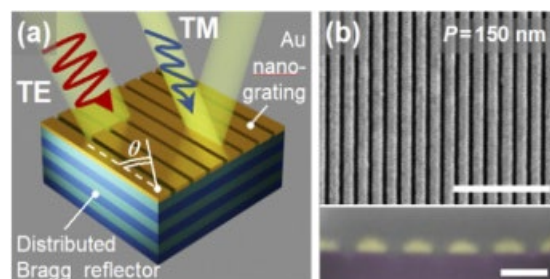


**Fig. 2.** (Left) SEM images of 3D columnar SiO<sub>2</sub> coatings over resist pillar patterns with different periods  $\Lambda = 0.8 \mu\text{m}$ ,  $1.3 \mu\text{m}$ ,  $3.1 \mu\text{m}$  and  $2.5 \mu\text{m}$ . (Right) Visualisation of retardance  $\Delta n \times H$  for different period patterns, hence, different thickness  $H$  as well as birefringence  $\Delta n$ . Stacked images were taken in a cross-Nicol setting with a sample at different orientation angles.

## Polarisation discrimination and surface sensing with a nanostructured hybrid mirror

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It was demonstrated experimentally how to turn a conventional distributed Bragg reflector into a polarization-selecting mirror operating in the near-IR at normal incidence without diffraction and with a high extinction ratio. Our approach combines a dielectric multilayer composite with a sub-wavelength metal wire-grid nanograting, which can be routinely fabricated using well-established planar fabrication techniques. Moreover, the design and working principle of the nanostructured hybrid mirror enable it to operate as a surface sensor and allow straightforward integration of the mirror with functional materials for tuning its wavelength/polarisations extinction ratio (Fig. 3).



**Fig. 3.** Polarisation-sensitive hybrid metal-dielectric mirror. (a) Schematics of the hybrid mirror interacting with normally incident linearly polarised light. Angle  $\theta$  shows the azimuth of incident polarisation. (b) SEM images of Au wire-grid nanogratings with periods of  $150 \text{ nm}$  fabricated on top of a conventional distributed Bragg reflector. The scale bar is  $150 \text{ nm}$ .



## Quality and flexural strength of laser-cut glass: classical top-down ablation versus water-assisted and bottom-up machining

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The growing applicability of glass materials drives the development of novel processing methods, which usually need a more comprehensive comparison to conventional or state-of-art ones. Our research compares the traditional top-down laser ablation methods in the air (TDC) to those assisted with a flowing water film (WTDC) using picosecond pulses. Furthermore, the bottom-up cutting method using picosecond (ps-BUC) and nanosecond pulses (ns-BUC) was also investigated. The laser-cut glass surface chipping, sidewall roughness and flexural strength were compared for various laser-cutting techniques. The smallest surface chipping up to 51  $\mu\text{m}$  was obtained for the WTDC technique. As for the side wall roughness, the TDC technique also showed the best results ( $R_a=0.28\ \mu\text{m}$ ). In the case of sample flexural strength, WTDC technique performance was evident, with a mean flexural strength

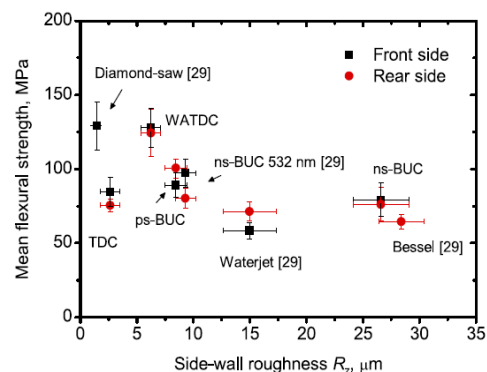


Fig. 4. The mean flexural strength versus average peak-to-valley distance ( $R_z$ ) of non-etched sidewalls.

of 134 MPa. Despite the advantages of TDC and WTDC techniques, bottom-up technology allowed us to achieve higher cutting speed and taper-less sidewalls, and was preferable for thick glass processing.

## Transversal and axial modulation of axicon-generated Bessel beams using amplitude and phase masks for glass processing applications

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The control of laser-induced microcracks in the volume of transparent materials is essential for scribing processes. The effect of various amplitude and single-level phase masks on both transverse and axial intensity distribution of the conventional axicon-generated Bessel beams was investigated. We demonstrated the volumetric crack control induced by an asymmetrical central core with an appropriately selected intensity level to avoid the influence of peripheral intensity maxima. Proper alignment of cracks and intra-distance between the modifications results in reduced separation stress of the scribed samples. Additional amplitude modulation of the incident Gaussian beam was introduced to flatten the axial intensity distribution of the axicon-generated Bessel beam.

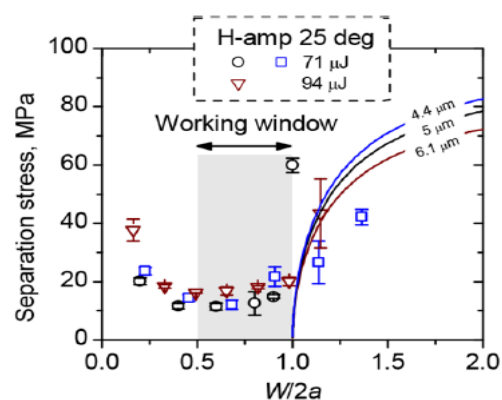


Fig. 5. Dependence of the separation stress on the ratio of the pitch to the full crack length.

## Laser-assisted surface activation for fabrication of flexible non-enzymatic Cu-based sensors

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A rapid and effective technique has been developed for the fabrication of sensor-active copper-based materials on the surface of such flexible polymers as terephthalate, polyethylene naphthalate (PEN) and polyimide using the method of laser surface modification. We optimised the polymer surface activation parameters using picosecond laser pulses for subsequent selective metallisation within the activated region. The fabricated copper structures were modified with gold nanostructures and by electrochemical passivation to produce copper-gold and oxide-containing copper species, respectively. As a result, compared to pure copper electrodes, these composite materials exhibit much better electrocatalytic performance, including the non-enzymatic identification of biologically important disease markers such as glucose, hydrogen peroxide and dopamine.

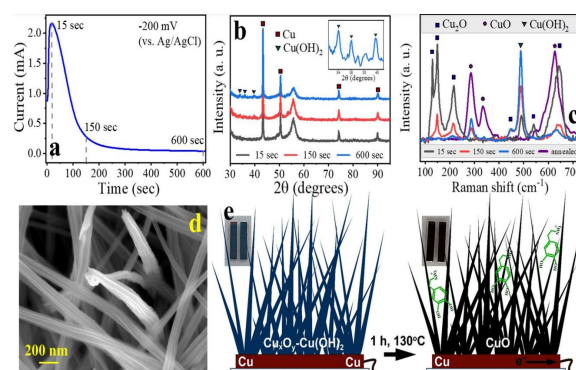


Fig. 6. (a) Amperometric curve recorded after passivation of copper deposits on the surface of PEN, (b) XRD patterns, (c) Raman scattering spectra of  $\text{Cu}_2\text{O}$ - $\text{Cu}(\text{OH})_2$  nanowires on the surface of the fabricated copper electrode, (d) SEM image of the  $\text{CuO}$  nanowires on the surface of the fabricated copper electrode after annealing, and (e) a schematic illustration of the modification process.

## Magnetic field-assisted wakefield generation and electron acceleration by Gaussian and super-Gaussian laser pulses in plasma

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Theoretical and experimental investigation of charged particle acceleration by lasers in vacuum and plasma is an exciting area of research due to its significance in various industrial and medical applications. Recently, to study this process, a number of models have been proposed and developed. We focus on electron acceleration and wakefield produced by Gaussian and super-Gaussian (SG) laser pulses through plasma medium in the attendance of an external magnetic field. It was observed, that increasing plasma electron density increases the amount of wakefield for SG laser pulse and decreases the wakefield of Gaussian laser pulse. The lower densities exhibit the larger electron bunch, and while the background electron density is altered, the amplitude of the wakefield changes. Besides, it was found that increasing plasma electron density leads to a decrease in the pulse duration compared to the SG laser pulse, and consequently, to weaker perturbations in the plasma electron density of the Gaussian laser pulse. As a result, the wakefield of the Gaussian laser pulse decreases compared to the SG one.

## Control of the wetting properties of stainless steel by ultrashort laser texturing using multi-parallel beam processing

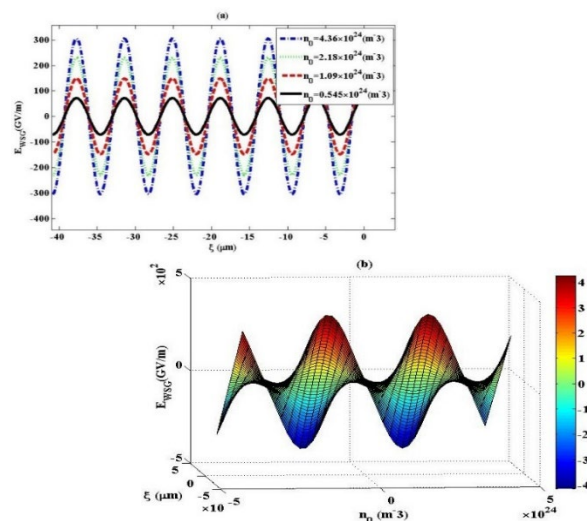
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Laser surface micro-texturing is increasingly used to produce surfaces with desired wetting characteristics. For this, not only precise but also fast laser processing is needed. Micro-textures not based entirely on laser-induced material self-organization require relatively tight focusing of the laser beam, which cannot be achieved using fast beam scanning systems. Therefore, the possibility of using parallel laser processing by a multi-beam array to control the EN 1.4301 stainless steel surface was investigated. High-energy picosecond laser pulses were used to pattern the polished steel surface using an  $8 \times 8$  beam array with two different patterning strategies: mesh and dot. It was determined that multi-beam mesh patterning allows to obtain superhydrophobic surface properties through the right combination of texture depth, surface chemical properties and laser-induced surface ripples. The dot

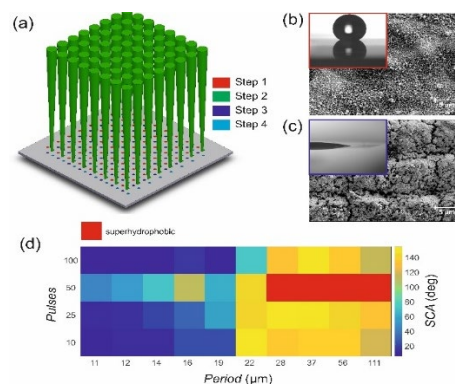
## Large-area fabrication of LIPSS for wetting control using multi-parallel femtosecond laser processing

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Control of surface properties such as wettability is an area of considerable interest. Material self-organization in a form of laser-induced periodic surface structures (LIPSS) could be a way to achieve wettability control. Formation of LIPSS requires relatively low laser fluence. However, to produce high regularity structure, a small laser spot size still has to be used to avoid loss of cohesion over the laser spot. In such a case, using parallel laser processing in which the desired pattern is created in a large area simultaneously is beneficial. Patterning was performed on a polished EN 1.4301 steel surface using an array of 64 beams attained using a diffractive element. Area scanning with an  $8 \times 8$  beam array was used to produce LIPSS in a large area during a single scanning process. The dependence of the LIPSS period on the hatch distance and

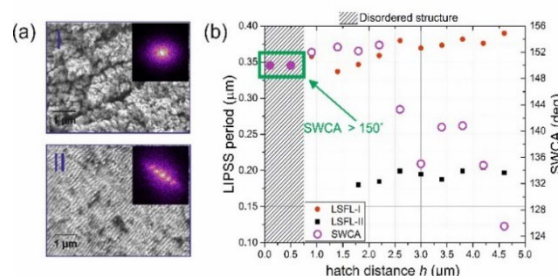


**Fig. 7.** (a) Variation of the wakefield with respect to distance for SG laser pulse and (b) 3-D diagram of a variation of  $E_{WSG}$  with respect to  $\xi$  and  $n_0$ . The chosen parameters are:  $B_0=45\text{T}$ ,  $I_0=2.14 \times 10^{22} \text{ W/m}^2$  for different values of  $n_0=0.545 \times 10^{24} \text{ m}^{-3}$ ,  $1.09 \times 10^{24} \text{ m}^{-3}$ ,  $2.18 \times 10^{24} \text{ m}^{-3}$  and  $4.36 \times 10^{24} \text{ m}^{-3}$ .



**Fig. 8.** (a) Fabrication of the dot structure using laser beam array. SEM images of (b) superhydrophobic and (c) superhydrophilic surface structures on steel, produced using multi-beam laser processing (inserts show water drops deposited on the respective surface). (d) Dependence of the static contact angle of the water droplet on the number of laser pulses and pattern period used in processing.

patterning was even more promising, and it was found to be suitable for obtaining a broad spectrum of wetting states ranging from superhydrophobic to superhydrophilic when appropriate patterning parameters were used.



**Fig. 9.** (a) SEM micrographs of the steel surface laser patterned using various hatch distance (laser spot overlap) values, where each SEM micrograph inset shows its 2D-FFT image. (b) Dependence of the LIPSS period and SWCA value on the hatch distance  $h$ .

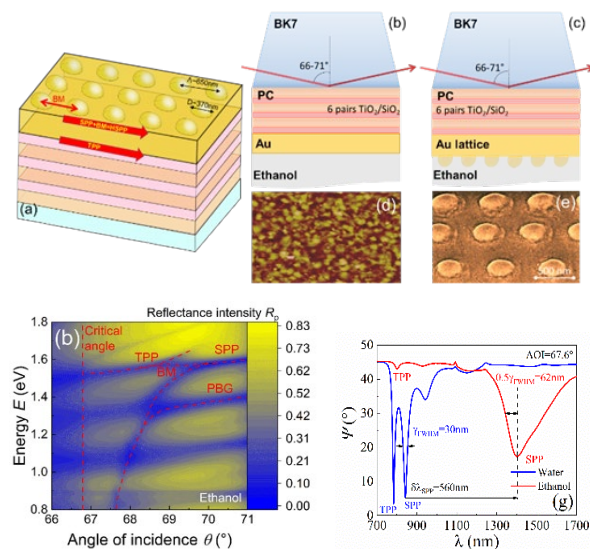
irradiation fluence was evaluated. Relationship between the static water contact angle and the structure parameters in the Fourier plane of the SEM micrographs was investigated.



## Influence of gold surface lattice array on the optical and sensing properties of the strongly coupled Tamm and surface plasmon polariton mode

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The total internal reflection ellipsometry (TIRE) method was used for the excitation and study of strong coupling between Tamm plasmon polariton (TPP) and surface plasmon polariton (SPP) in nanophotonic structures with 1D photonic crystal (PC) and lattice of gold nano-bumps. The changes induced by periodic gold surface lattice give longer propagation length for the SPP component and decreasing propagation length for the TPP. The results demonstrate a novel approach to control and change of the propagation length under a strong coupling regime between TPP and SPP components in the hybrid plasmonic mode using surface lattice arrays. Very high hybrid plasmonic mode sensitivity  $S_{\text{HSPP}} \approx 26000 \text{ nm/RIU}$  compared to the refractive index on the uniform gold layer was shown. The sensitivity to the ellipsometric parameters  $\Psi$  and  $\Delta$  on the gold lattice was relatively high due to the increased Q-factor of the resonances. Comparison of plasmonic resonance sensitivity to the refractive index changes of hybrid TPP-SPP mode on the uniform gold layer and traditional SPP, has shown that the hybrid plasmonic mode overcomes the SPP mode by about 27%. Applying surface lattice resonances together with a strong coupling regime, leads to decrease of losses, resulting in the increase of propagation length and better coherence properties of such plasmonic excitations. This, in turn, promises advanced properties for the threshold-less plasmonic-based nanolasers and advanced optical biosensors.

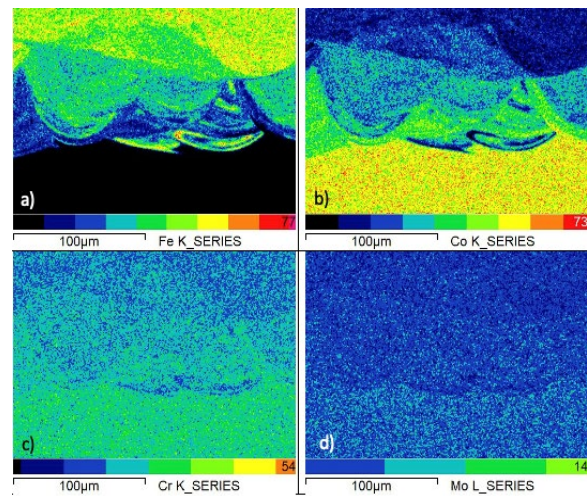


**Fig. 10.** Top: (a) structure consisting of gold nano-bumps lattice with a diameter of  $\sim 370 \text{ nm}$  and a period of  $\sim 652 \text{ nm}$ . Schemes of excitation configurations for hybrid (b) TPP-SPP and (c) SPP-HSPP modes. (d) The SEM micrograph of uniform (50 nm) Au layer and (e) an array of nano-bumps lattice on the same thin gold layer. Bottom: (left) reflectance intensity of p-polarized light as a function of energy vs incident angle for lattice array of gold nano-bumps; (right) spectra of ellipsometric parameter  $\Psi(\lambda)$  in water and ethanol for 1D PC and a uniform gold layer.

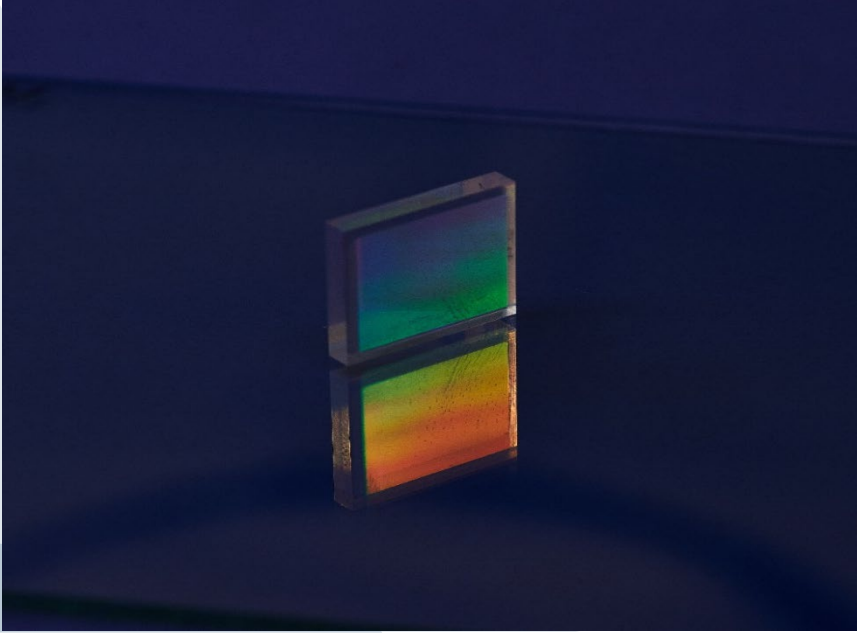
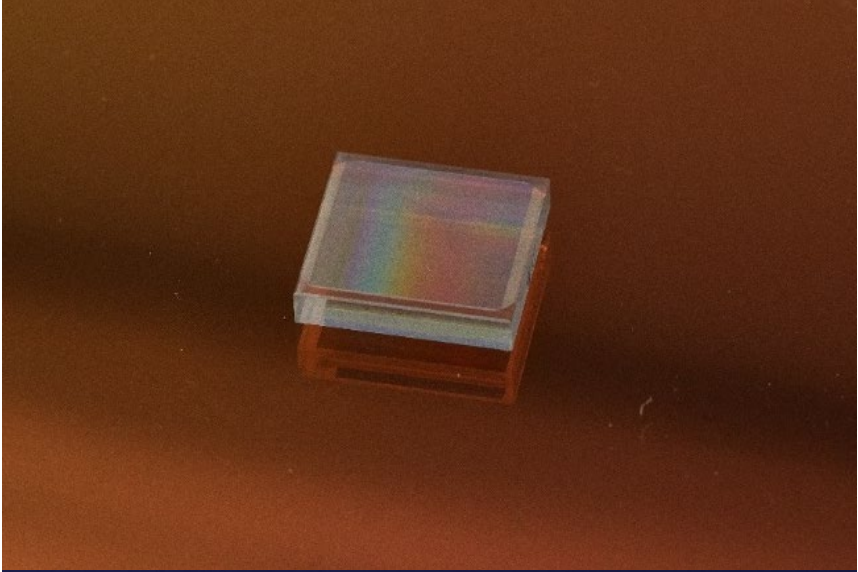
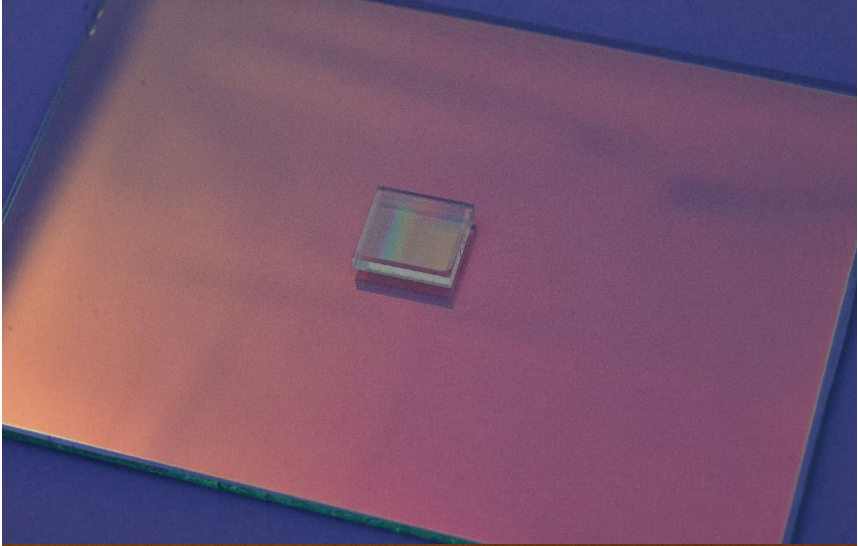
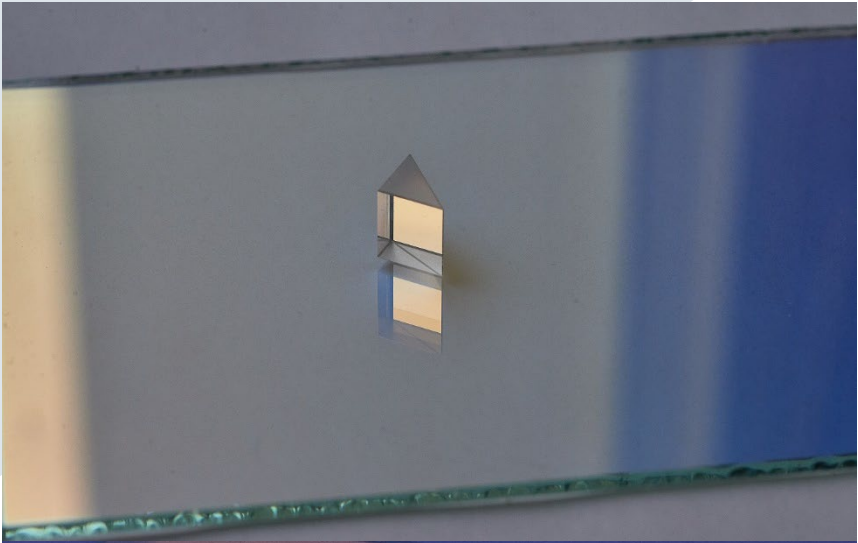
## Bimetallic structure formation by laser powder bed fusion

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Using laser powder-bed fusion (L-PBF) additive manufacturing, bimetallic structures can be produced by depositing different materials in a layer-by-layer fashion. The L-PBF bimetallic structure was created by combining 17-4 PH stainless steel and CoCrMo alloy. By using these two materials, it was possible to improve the hardness and corrosion resistance of the alloy and retain magnetic properties – a characteristic of the 17-4 PH stainless steel. A sandwich-like bimetallic specimen was manufactured, and its fusion zone was analysed. The morphology, element distribution and hardness of the fusion zone were investigated. A gradual change in chemical element distribution was observed at the two-material fusion zone. The thickness of the fusion zone was around  $400\text{--}450 \mu\text{m}$ . The hardness of the fusion zone ( $104 \pm 2 \text{ HRB}$ ) was higher than the hardness of 17-4 PH ( $95 \pm 2 \text{ HRB}$ ) but lower than CoCrMo ( $111 \pm 2 \text{ HRB}$ ). The experimentally evaluated density of the bimetallic specimen was  $8.01 \text{ g/cm}^3$ . The difference in values proves that the fusion zone of the specimen possesses unique characteristics that are not specific to either of the materials.

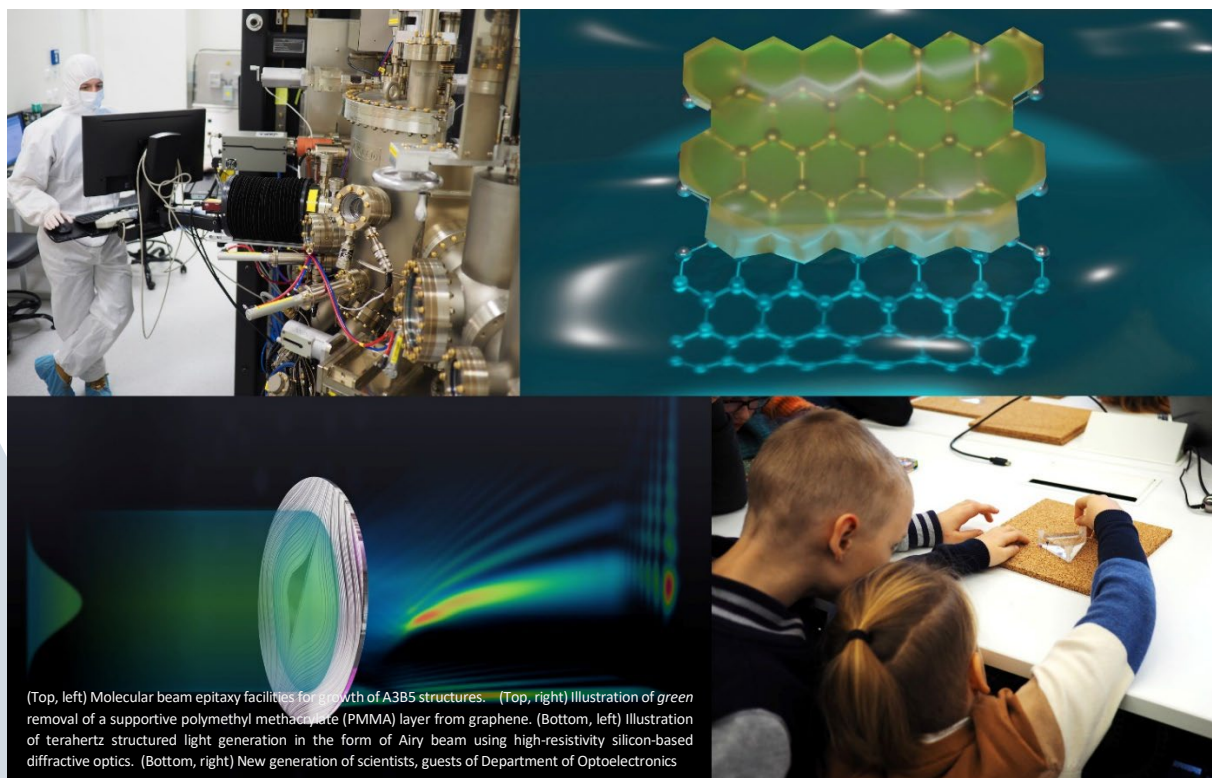


**Fig. 11.** SEM-EDS maps showing (a) Fe, (b) Co, (c) Cr and (d) Mo elemental distribution.





# Optoelectronics



(Top, left) Molecular beam epitaxy facilities for growth of A3B5 structures. (Top, right) Illustration of green removal of a supportive polymethyl methacrylate (PMMA) layer from graphene. (Bottom, left) Illustration of terahertz structured light generation in the form of Airy beam using high-resistivity silicon-based diffractive optics. (Bottom, right) New generation of scientists, guests of Department of Optoelectronics

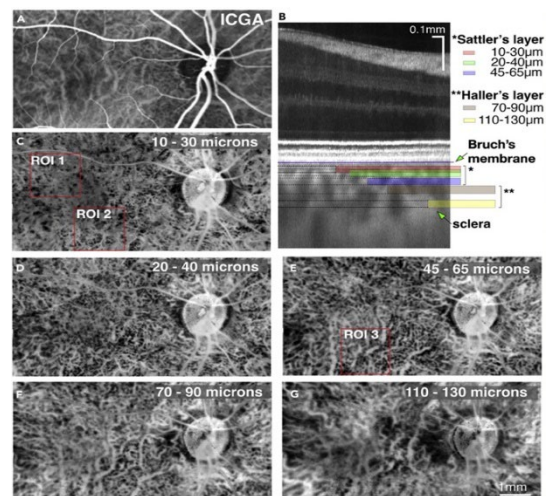
## Spotlight on terahertz and infrared ranges: from scientific idea up to innovative prototypes and technologies

Department of Optoelectronics which consists of five scientific laboratories (Ultrafast Optoelectronics, Optoelectronics Technology, Semiconductor Optics, Terahertz Photonics and Optoelectronics Systems Characterization) concentrates on two main scientific directions. The first one is dedicated to the development of terahertz (THz) technologies, in particular, to imaging and spectroscopy, their tools and applications. The second direction relies on materials engineering and their investigation for fabrication of infrared range devices. The core technology behind the fundamental and applied research is molecular beam epitaxy (MBE) for A3B5 nanostructures grown employing two apparatus produced by SVT and Veeco companies. The scientific activities cover design and investigation of quantum wells of GaAs/AlGaAs and GaInAsBi compounds, development of infrared light emitting diodes (LEDs) and lasers based on these structures, as well as solar cells based on novel semiconductor nanostructures. The year 2022 was successful in further evolution of mentioned investigations and applications. The topic of fabrication of several-atom-thick layers of Bismuth (Bi) - bismuthene was one of important achievements. We discovered that it can behave not only as a semiconductor, but also as a topological insulator at room temperature. Infrared LEDs based on GaInAsBi quantum wells were designed, fabricated and investigated this year. Particular attention was also paid to development and study of triple junctions containing AlGaAs/GaAsBi compounds for solar cell applications. Experimental facilities of THz investigations are concentrated in the interlaboratory unit of the Department called THz photonics and technology Cluster. The available equipment containing various THz techniques, femtosecond laser-based THz spectrometers, as well as different continuous wave-based THz set-ups for imaging, standard optical characterization techniques (photoluminescence, modulation spectroscopy, Fourier spectroscopy, optical and THz ellipsometry), equipped with low-temperature facilities and possibility to apply short-pulse electric fields, were successfully employed. In particular, we invented a novel scalable and green method to remove the supportive polymethyl methacrylate (PMMA) layer from graphene and obtained promising results for GaN with a huge potential for applications. Also, noteworthy are the groundbreaking results for GaAs/AlGaAs superlattices, dedicated to dissipative parametric gain effects of high frequencies, as well as structured THz light generation and its application in lensless THz imaging systems. At last, but not least, a breakthrough scientific achievement should be mentioned in optical coherence tomography for non-invasive human retinal volumetric imaging in vivo, advancing the detection, diagnosis, and monitoring of various retinal diseases.

## Spatio-temporal optical coherence tomography provides full thickness imaging of the chorioretinal complex in human eye *in vivo*

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Optical Coherence Tomography (OCT) has been successfully used for non-invasive diagnostics and monitoring of various human retinal diseases *in vivo*. However, the spatial resolution, imaging speed and depth is still a major issue in OCT that prevents clear imaging of various retinal and choroidal layers. Recently, to speed up OCT imaging, a new approach based on a superfast camera and a swept laser source has been introduced. We have optimized this technology by (a) employing a multimode fiber for coherent noise reduction in OCT images and (b) introducing a line camera to facilitate patient alignment and imaging. Fig. 1 shows that the developed system enables acquisition of retinal and choroidal layers with high contrast and resolution, achievable only with Adaptive-Optics OCT. It demonstrates the potential of the technology for a non-contact method in clinical use.

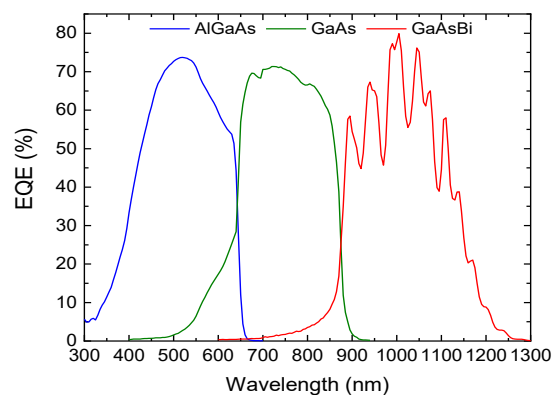


**Fig. 1.** (A) ICG angiography image for comparison purposes, exposing mostly large vessels of Haller's layer. (B) A cross-sectional image-map (with indicated layers). (C–G) Contrast-inverted OCT images generated at different depths (as indicated in each image).

## Triple junction AlGaAs/GaAsBi solar cells

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The Optoelectronics technology laboratory focuses on the molecular beam epitaxy of group III-V alloys and superlattices for infrared range device applications. Among novel semiconductor alloys, the dilute bismide GaAsBi has drawn attention worldwide due to its favorable bandgap energy tuning properties. We developed a prototype thin film triple-junction AlGaAs/GaAs/GaAsBi solar cell, which incorporates bismide as the 1.0 eV bandgap bottom subcell. The results of external quantum efficiency (EQE) measurement of the solar cell are shown in Fig. 2. This marks the first GaAsBi-based multi-junction solar cell ever developed. The incorporation of GaAsBi in the triple-junction device was made possible using a metamorphic InGaAs buffer layer which allowed to achieve a thick high-quality GaAsBi alloy. During the development, a record-setting standalone 1.0 eV GaAsBi subcell was also produced.

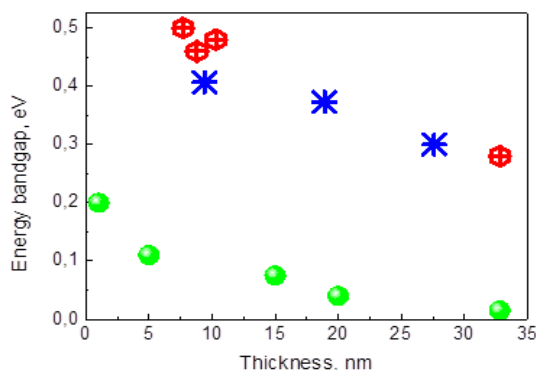


**Fig. 2.** External quantum efficiency graph of GaAsBi-based thin film triple-junction solar cell.

## Thin means interesting

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First quantum wells from solid-state material were made of bismuth layers in 1965. It was shown that quantum confinement of electrons takes place in a layer of about 50 nm thick, and Bi turns from a semimetal to semiconductor. Attention to thin Bi layers has been revived by the success of their distant relative, graphene. It turned out that several-atom-thick layers of Bi - bismuthene – can be as semiconductor as well as a topological insulator at room temperature – featuring a new material important for the creation of quantum computers. We have grown 7 – 30 nm thick Bi layers on (111) oriented Si substrates by MBE. Depending on the substrate temperature, rhombohedral  $\alpha$ -Bi or hexagonal  $\beta$ -Bi layers were obtained. Using THz radiation excitation spectroscopy, the dependence of the direct bandgap of the layers on their thickness was found. The dependences of both phases were similar (Fig. 3), with the largest direct bandgap equal to 0.5 eV for 7 nm thick layers.



**Fig. 3.** Energy bandgaps of ultrathin Bi layers. Red hexagons –  $\alpha$ -Bi, blue stars –  $\beta$ -Bi. Green circles – indirect bandgap of Bi layers..



## Longer waves in quantum wells

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The most efficient semiconductor light sources are those that have quantum wells in their active regions. However, quantum confinement increases the energy of the electron levels, causing problems in creating long-wavelength light sources. To solve this problem, we used quantum wells from bismide layers. This material is unique because the off-set of its conduction band with other A3B5 group semiconductors is small, so it is possible to realize a situation where electrons and holes are confined in quantum wells of different widths - the former in a wide one, the latter in a narrow one, and the energy levels of both charge carriers will change minimally (Fig. 4). There were MBE-grown GaInAsBi quantum wells with additional GaInAs layers on both sides; it was experimentally determined that the emitted wavelength of LEDs with such composite quantum wells reached  $2.6\ \mu\text{m}$  – as much as  $0.5\ \mu\text{m}$  longer than of LEDs with conventional quantum wells.

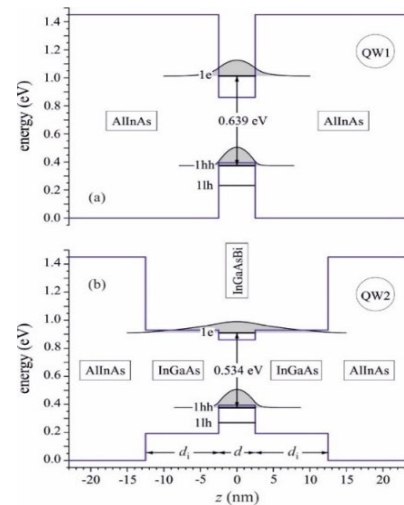


Fig. 4. Energy band structure of (a) conventional and (b) composite quantum wells.

## Dissipative parametric amplification of GHz frequencies in GaAs/AlGaAs superlattices

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Lack of compact powerful emitters is essential obstacle preventing evolution of THz imaging systems and their applications stimulating a novel concept to generate/amplify the radiation. Here we have demonstrated that subcritically doped quantum semiconductor GaAs/AlGaAs superlattice tuned to the Esaki-Tsu regime can successfully be employed for parametric gain of high frequency radiation at room temperature. We argue that the electric field component of the microwave pump wave, directed along the superlattice axis  $z$ , as shown in Fig. 5, parametrically interacts with the miniband electrons and excites a dozen of growing waves at frequencies satisfying the parametric conservation for photons. The generated longitudinal electrostatic waves propagate along the superlattice axis at the electron drift velocity before being converted to radiation through the wire antenna. The excitation of such slow electrostatic waves in the superlattice provide a significant enhancement of the gain in the order of  $\approx 10^4\ \text{cm}^{-1}$  and enables multiphoton generation in the cavityless configuration.

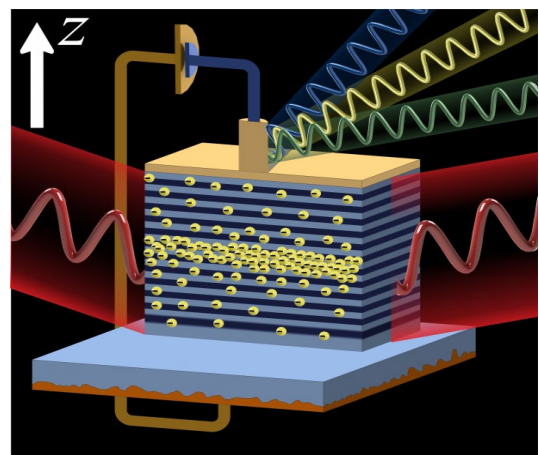


Fig. 5. Schematic illustration of the parametric gain in the GaAs/AlGaAs superlattice.

Our experiments confirmed core predictions of the existing theory of dissipative parametric amplification at GHz frequencies, and also further stretched its limits by describing the multiple parametric processes.

## Structured terahertz light for imaging and materials inspection

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It was demonstrated that THz structured light – electromagnetic waves with strongly displayed spatial inhomogeneity of amplitude, phase, and polarization – can be generated in a compact way using exclusively silicon diffractive optics prepared by femtosecond laser ablation technology. It was shown that THz structured light in imaging consistently outperforms the conventional approach in resolution and contrast, thus opening new frontiers of structured light applications in imaging and materials inspection. It enables sophisticated estimates of optical properties of novel materials, for instance, such 2D materials as graphene. For this aim different samples with different numbers of graphene layers were deposited on silicon substrate which is transparent to THz light and interacts with the wafer. It was evidenced that electron depletion and mechanical strains inducing change in graphene optical properties, can be nicely resolved employing features of THz structured light.



Fig. 6. Photo (main body) of Airy lens for THz structured light generation. Inset – schematic illustration of the lens performance.

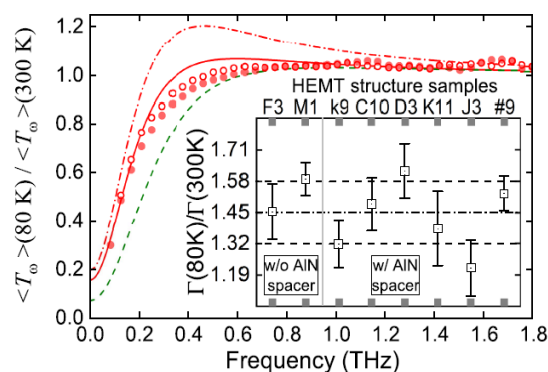
It is known that non-diffracting electromagnetic radiation displays an ability to self-heal and reconstruct after being met with an obstacle. As Airy illumination has a self-accelerating bending propagation trajectory, it was expected to observe its ability to illuminate an object behind an obstacle, e. g. to see an object placed behind the corner. The performed experiment confirmed this ability.

## GaN devices for THz photonics and electronics

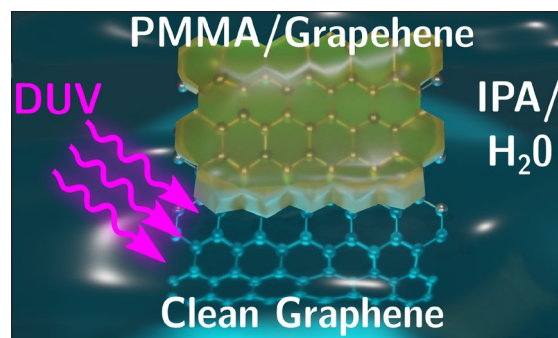
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Since 2014, we have been working on various nitride-based semiconductors developing custom-designed devices for THz photonics and electronics. Recent research was devoted to the development of a quaternary lattice matched (LM) InAlGa<sub>N</sub> barrier high electron mobility transistor (HEMT) structures. It showed a thermally stable density of two-dimensional electron gas (2DEG) equal to  $1.2 \times 10^{13} \text{ cm}^{-2}$  with the values of low-field mobility 1590  $\text{cm}^2/\text{V/s}$  and 8830  $\text{cm}^2/\text{V/s}$  at 300 and 77 K temperature, respectively. The X-ray diffraction data and modeled band diagram characteristics revealed the structure  $\text{In}_{0.165}\text{Al}_{0.775}\text{Ga}_{0.06}\text{N}/\text{Al}_{0.6}\text{Ga}_{0.4}\text{N}$ , with the parameters explaining the origin of barrier photo-luminescence peak position at 3.98 eV, linewidth of 0.2 eV and expected red-shift of 0.4 eV. The self-heating effects of annealed Ti/Al/Ni/Au ohmic contacts and 2DEG in AlGa<sub>N</sub>/Ga<sub>N</sub> HEMTs were investigated under strong electric fields. The contact self-heating with the increase of electric current was found to dominate over the 2DEG performance even under short-duration (only 100 ns) and low-duty-cycle (only  $10^{-5}$ ) pulse regime. The thermal renormalization of the 2D electron effective mass in commercial AlGa<sub>N</sub>/Ga<sub>N</sub> HEMT structures was observed by THz time domain spectroscopy (TDS) of Drude conductivity. The 1.45-fold mass increase was found to compare with its nominal value obtained at cryogenic temperatures (Fig. 7).

Green, scalable method to remove a supportive polymethyl methacrylate (PMMA) layer from the CVD graphene was proposed recently. First, the polarity of PMMA was modified with deep-UV irradiation. Next, rapid and complete dissolution of photo-exposed PMMA was performed in environmentally friendly mixture of alcohol and water. Independent comprehensive measurements revealed a good material quality and a high charge carrier mobility in the CVD graphene obtained by our new method. The fabrication of recessed electrical elements by direct laser ablation was proposed for microelectronic industry of wide-band gap semiconductors and HEMT devices (patent EP3975224B1).



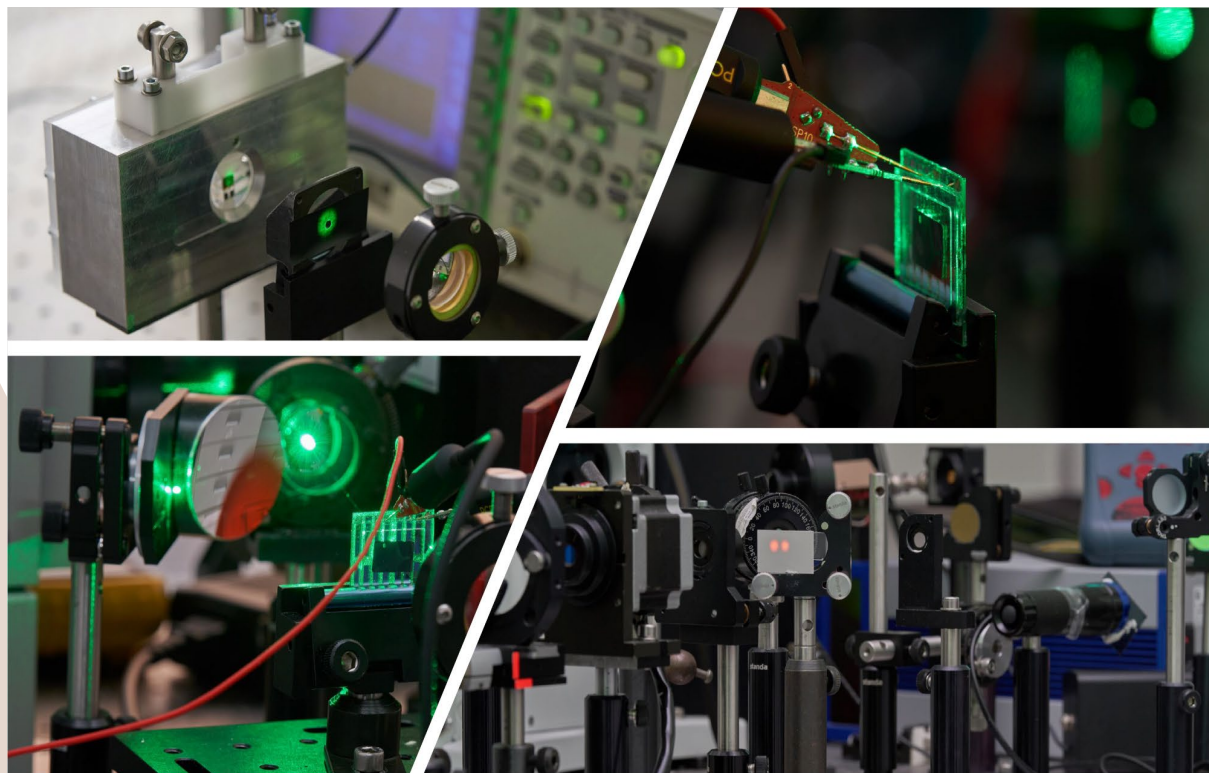
**Fig. 7.** Ratio of transmission characteristics of the AlGa<sub>N</sub>/Ga<sub>N</sub> HEMT structures: measured (solid symbols) and modeled under assumption that the electron effective mass at 300 K was of  $0.22m_e$  (dot-dashed line) and  $0.34m_e$  (solid line). Inset: average values of the radiative decay rate ratios of various HEMT structures demonstrate the up to 1.45 fold increase of  $m_e$  at 300 K.



**Fig. 8.** Green removal of a supportive polymethyl methacrylate (PMMA) layer from the CVD graphene by using our new patented method.



# Molecular physics



## Department of Molecular Compounds Physics

The activity of the Department of Molecular Compounds Physics is related to molecular photonics ranging from development of advanced optical and optoelectrical materials characterization techniques to the investigation of natural and artificial molecular systems, development of molecular and hybrid devices. We seek for better understanding of photoinduced processes in molecular, hybrid systems and nanostructures, optimization of the material properties and processes in photonic devices. Unlimited variety of organic molecules, as well as a broad range of technological fabrication abilities promise a wide spectrum of device characteristics and their application fields. On the other hand, that raises requirements for a detailed understanding of molecular properties and photoinitiated processes. Various intramolecular and intermolecular interactions create complex hierarchical structures determining properties of molecular systems and their functional peculiarities. In addition to electrons and holes, excitons and ions play crucial roles in organic semiconductors, while relatively weak intermolecular interactions determine morphology of molecular materials and complex structures of biological systems. All this complexity has to be taken into consideration in order to enhance the efficiency of the molecular devices and to understand functions of molecular systems in nature. Advanced experimental techniques such as ultrafast spectroscopy, nonlinear and single molecule microscopy, optoelectrical methods are used together with theoretical calculations to address excited-state dynamics and progressions of electronic events. Objects of our investigation range from biological photosynthetic and protein-DNA complexes, molecular viscosity sensors, nanostructures for medical applications to organic and perovskite solar cells. This interdisciplinary research field requires expertise in physics, chemistry, biology as well as material and device engineering. Since it is difficult or even impossible to be excellent in all these research disciplines, our research is often based on collaboration with researchers from other Lithuanian and foreign academic and other high-tech institutions, which also helps us to be a part of the international research.

## Photoluminescence dynamics of MAPbI<sub>3</sub> perovskite films induced by lateral electric field

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The time-dependent behavior of perovskite devices is a limiting factor for widespread use of these materials for optoelectronic applications. The exact mechanisms underlying the dynamics of the device performance remain elusive. We show that by combining photoluminescence (PL) and electric field-induced second harmonic microscopy (EFISH) techniques, it is possible to image and identify voltage-induced lateral dynamic processes in methylammonium lead iodide perovskite thin films. We show a sequence of voltage-induced dynamic steps: i) appearance of a short-lived bright PL next to the positive electrode; ii) formation of a moving dark PL front; iii) appearance and blinking of bright PL spots; iv) growth and subsequent decay of the bright PL spots after voltage is turned off.

## All-optical thermometry with NV and SiV color centers in biocompatible diamond microneedles

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Monitoring of tiny intracellular temperature variations is of high importance to understand the mechanisms of exothermic/endothermic processes inside the living cells. Small shifts in thermal balance may drastically influence cell functioning and induce pathological conditions. By using biocompatible diamond single-crystal microneedles enriched with nitrogen-vacancy (NV)/silicon-vacancy (SiV) color centers, this study demonstrates all-optical in vitro temperature monitoring in the physiologically significant range (25–55 °C). This study demonstrates experimentally that temperature can be measured by lifetime, full-width at half maximum, and peak position of SiV zero-phonon line (ZPL), while accuracy can be further improved by normalizing the photo-luminescence (PL) ZPL peak intensity on the PL signal measured at the wavelength, where it is temperature independent.

## Structure-based model of FCP – the major light-harvesting complex of marine algae

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Diatoms are a group of marine algae that are responsible for a significant part of global oxygen production. Adapted to the life in aqueous environment dominated by the blue-green light, their major light-harvesting antennae–fucoxanthin–chlorophyll protein complexes (FCPs) – exhibit different pigment composition than that of plants. Using the crystallographic information of FCP complex from *Phaeodactylum tricornutum* diatom, obtained just in 2019, and quantum chemistry-based calculations, we constructed the structure-based excitonic Hamiltonian of FCP that is the basis for any modeling of stationary or time-resolved spectroscopic data. We also calculated the inter-pigment Förster energy transfer rates and identified two quickly equilibrating chlorophyll clusters.

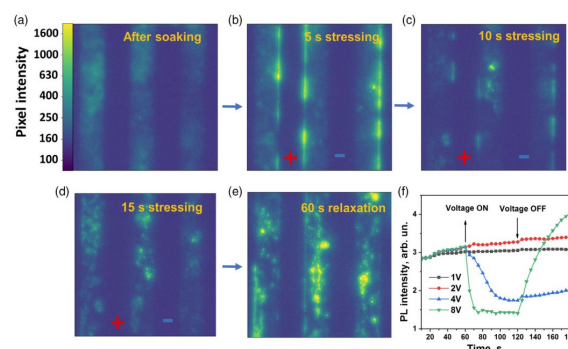


Fig. 1. PL images measured (a) before voltage application and (b–d) at different times after application of 8 V voltage; (f) dynamics of the integrated PL intensity under different applied voltages.

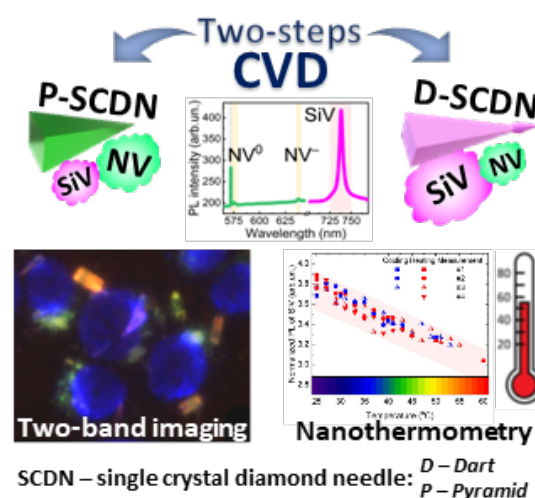


Fig. 2. Operation principle of diamond microneedles-based all-optical thermometry.

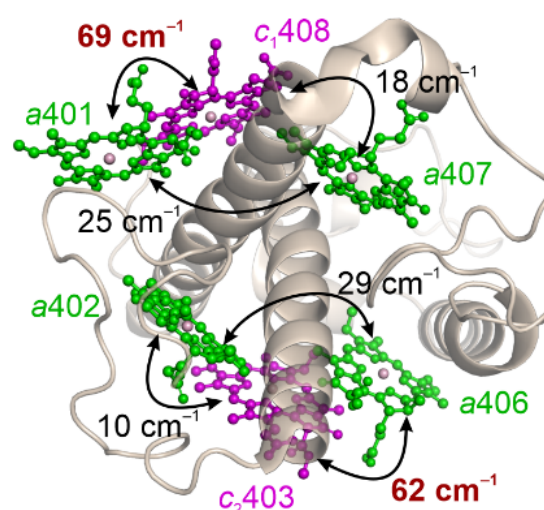


Fig. 3. The calculated largest excitonic couplings between chlorophylls of a-type (green) and c-type (magenta) in the FCP complex from *Phaeodactylum tricornutum* diatom.



## Carrier generation and recombination in all-organic solar cells

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Organic bulk heterojunction solar cells with electron acceptors based on small donor-acceptor type molecules show record efficiencies mainly due to their long wavelength absorption, which enables efficient harvesting of solar light and, thus, causes high current density. Meanwhile, relative positions of HOMO and LUMO levels of donor and acceptor materials determine the open circuit voltage. We applied ultrafast transient absorption and transient luminescence techniques together with specially-designed modelling technique to address charge carrier generation and recombination dynamics in detail. We demonstrate the importance of careful adjustment of the HOMO and LUMO levels, as their positions determine formation and recombination rates of interfacial charge transfer (CT) states. An insufficient donor and acceptor LUMO level offset (lower than  $\sim 300$  meV) leads to slow and inefficient CT state formation, while an offset of the HOMO level below  $\sim 100$  meV leads to fast CT state recombination due to the back transfer of the hole from donor to acceptor.

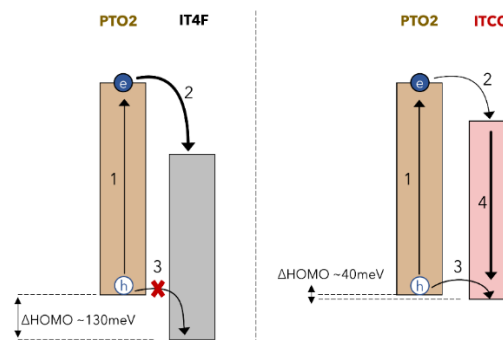


Fig. 4. Charge carrier generation and recombination scheme demonstrating role of the hole transfer (process 3) in carrier recombination via regenerated excited state of acceptor.

## Quantitative and qualitative analysis of PAH fibrosis using wide-field second harmonic generation microscopy

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We demonstrated that wide-field second harmonic generation (SHG) microscopy of lung tissue in combination with quantitative analysis of SHG images is a powerful tool for fast and label-free visualization of the fibrosis pathogenesis in pulmonary arterial hypertension (PAH). Statistical analysis of the SHG images revealed changes of the collagen content and morphology in the lung tissue during the monocrotaline-induced PAH progression in rats. First order statistics disclosed the dependence of the collagen overproduction on time, while the second order statistics indicated tightening of collagen fiber network around blood vessels and their spreading into the alveolar region. Fourier analysis revealed that enhancement of the fiber orientation in the collagen network with PAH progression was followed with its subsequent reduction at the terminating phase of the disease. The proposed approach has potential for assessing pulmonary fibrosis in interstitial lung disease, after lung(s) transplantation, cancer, etc.

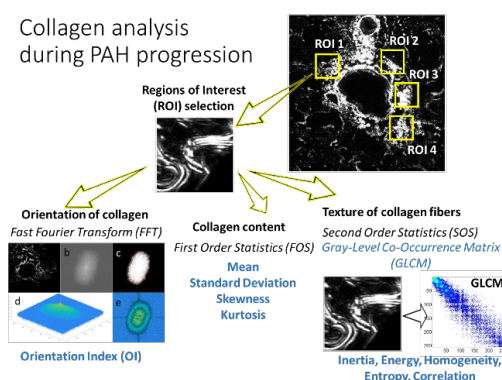


Fig. 5. The principal diagram of collagen analysis.

## Red fluorescent BODIPY molecular rotors for microviscosity, temperature and polarity sensing

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Mapping environmental properties in biosystems is an important capability that can aid in disease detection. This can be achieved using red fluorescent sensors based on BODIPY group. We report how electron-withdrawing (EWG) and electron-donating (EDG) groups can change the spectral and sensory properties of  $\beta$ -phenyl-substituted BODIPYs. Moreover, we show that nitro-substitution of meso-phenyl is a versatile approach to improve the sensitivity to viscosity while suppressing sensitivity to polarity and temperature. We also explain how the energy barrier height ( $E_a$ ) for non-radiative relaxation affects the probe's sensitivity to temperature and viscosity.

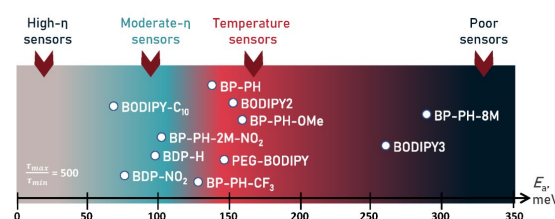
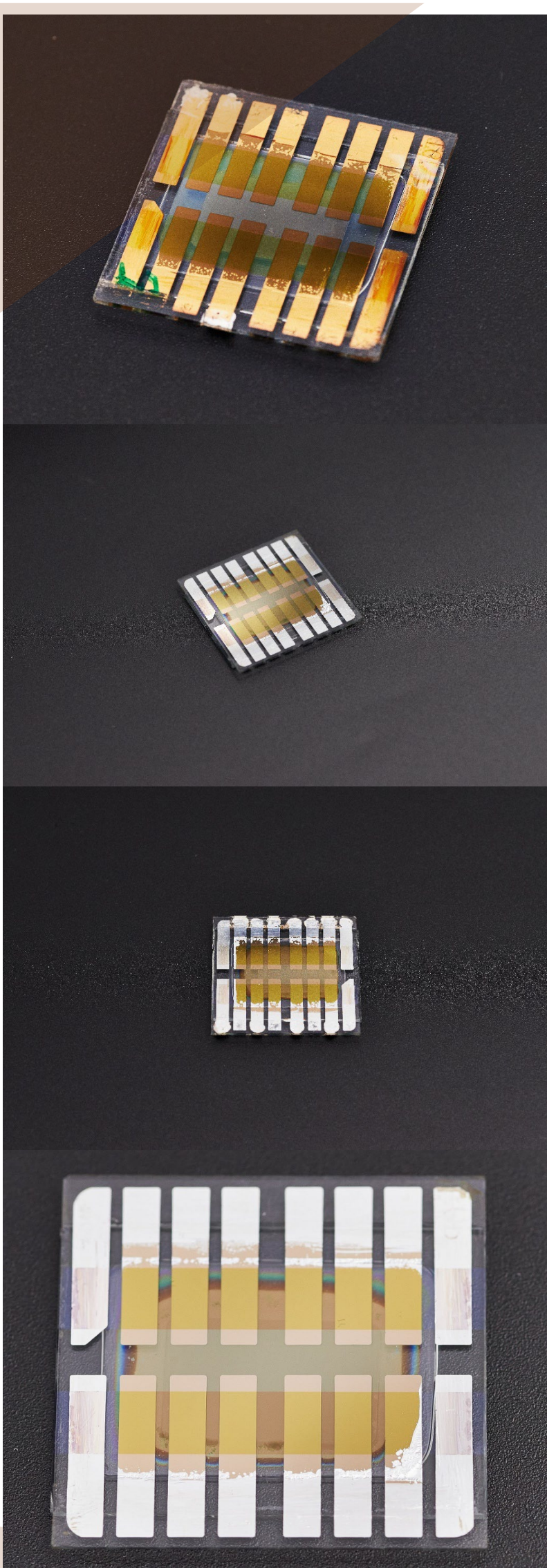
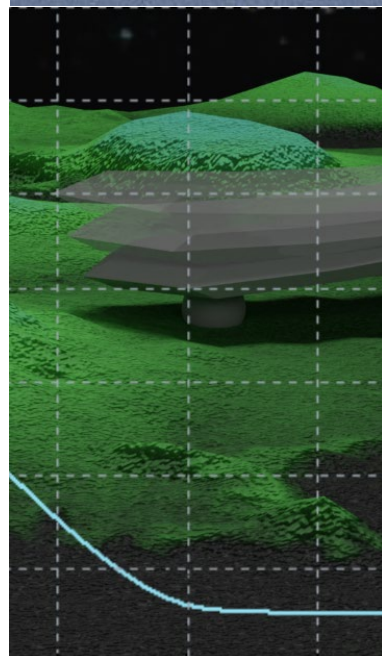
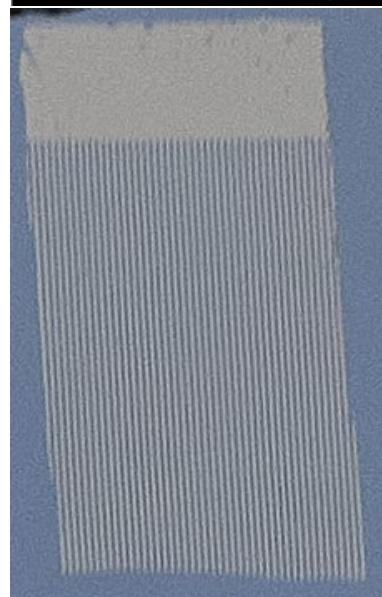
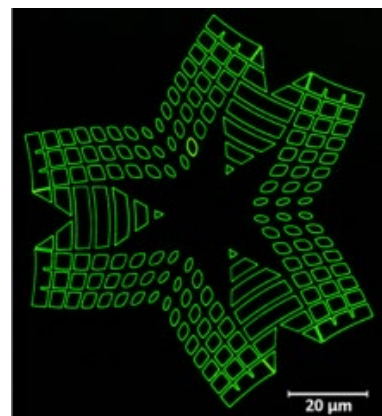
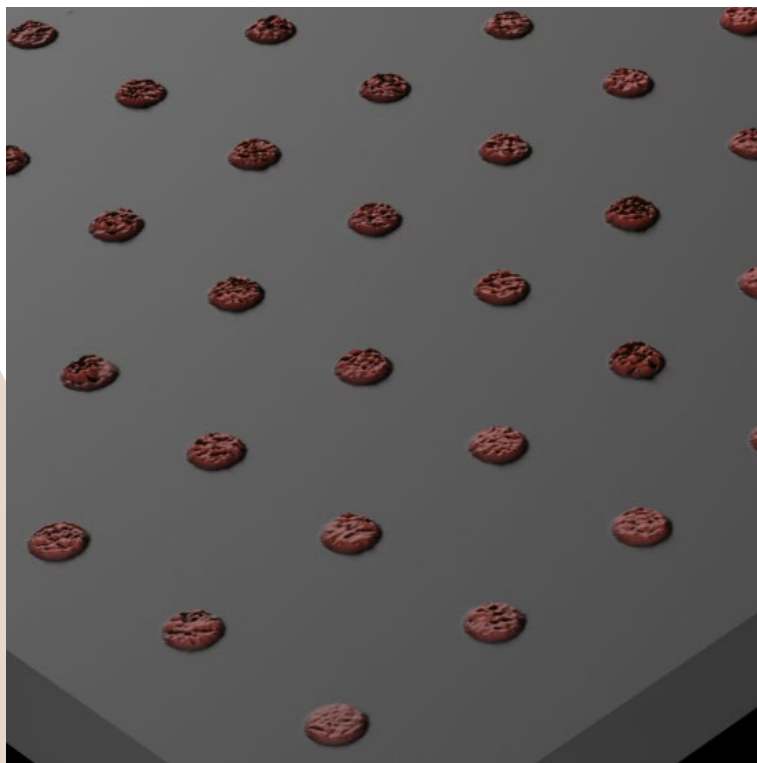


Fig. 6. Visual scale demonstrating energy barrier values for different types of sensors. From left: light grey—high-viscosity sensors, sky blue—moderate-viscosity sensors, red—temperature sensors, dark grey—poor sensors. White dots indicate energy barrier values of BODIPY derivatives.





# Nanoengineering



## The Department of Nanoengineering

An interdisciplinary research unit that focuses on the nanometer-scale material properties and phenomena at the interface between solid and soft matter, synthetic and biological materials as well as develops novel fabrication and analysis techniques. The competence of the team spans the fields of surface chemistry, molecular biophysics, organic synthesis and supramolecular chemistry, laser technologies, scanning probe and fluorescence microscopy, electrochemistry, as well as cell biology and tissue engineering. The experimental and technological capacities can be grouped as follows:

- ▣ Ultrathin organic coatings and functional modifications of solid and soft material surfaces,
  - ▣ Alternative microfabrication based on soft lithography and inkjet printing,
  - ▣ Scanning probe nanolithography, rapid prototyping of solid, organic, biological and hybrid nanostructures,
  - ▣ Synthesis of (bi)functional compounds, bioconjugates, self-assembling blocks,
  - ▣ Electrochemical sensing, carbon nanomaterials, nanoparticle and microfabricated electrodes,
  - ▣ Advanced atomic force microscopy and force spectroscopy,
  - ▣ Real time molecular interaction analysis, surface plasmon resonance,
  - ▣ Biochip technologies, biomaterial characterization, 2D and 3D cell culture, Automation, electronics, hardware and equipment development.
- The department is open for both scientific and industrial collaborations, it regularly provides services to SMEs as well as global companies.

## An electrochemical sensor for dopamine based on thermally reduced graphene oxide

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Modification of the thermal reduction of graphene oxide (GO) was improved by adding malonic acid and  $P_2O_5$  of preoxidized natural graphite. These new rGO samples showed incorporation of P functional groups into the structure of rGO as evidenced by XPS and Raman spectroscopy. Electrochemical characterization revealed more capacitive behaviour of rGO compared to graphite. In particular, one of the obtained materials, which was preoxidized in the presence of  $H_2SO_4$ ,  $HNO_3$ , and  $Cr_2O_3$ , increased the sensitivity to the electrochemical redox performance of dopamine (DA). The DA oxidation peak current was much higher than that of unmodified glassy carbon or graphite electrodes, thus improving the sensitivity to this neurotransmitter. The best limit of detection was 110 nM and the sensitivity was  $28.64 \mu A \mu M^{-1} cm^{-2}$ . The advantages of such an electrochemical sensor are fabrication without additional electron transfer mediators, long stability (at least for one month) and good selectivity.

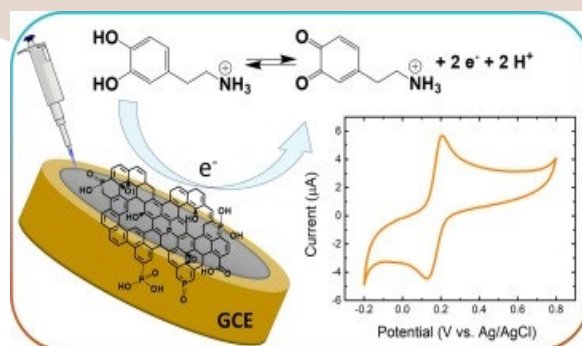


Fig. 1. Scheme of the dopamine sensor development using thermally reduced graphene.

## Novel electrochemical pH monitoring based on polyfolate

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Conducting polymer polyfolate (PFA) was electrochemically synthesized on a pyrolytic graphite electrode (PGE) covered with chitosan (Chit). It is known that folic acid is pH sensitive in the range between 6 and 10. In the optimal approach Chit was drop cast on PGE and then PFA was polymerized from folate monomer in 0.1 M phosphate buffer saline solution of pH 6.0. Microscopic characterization revealed that PFA is synthesized and forms clusters on Chit-coated graphite electrodes. The surface coverage was determined to be from 52 to 183 nmol  $cm^{-2}$  depending on pH. A capacitive behaviour was observed from the electrochemical impedance spectra for the sensor in the negative potential region, while at higher positive potentials, i.e. + 1.0 V, it was resistive due to the charge transfer. The novel PFA/Chit/PGE electrode was sensitive to pH from 6.0 to 9.0 with a sensitivity of  $43.5 \pm 1.5$  mV/pH and stability of over 70 days.

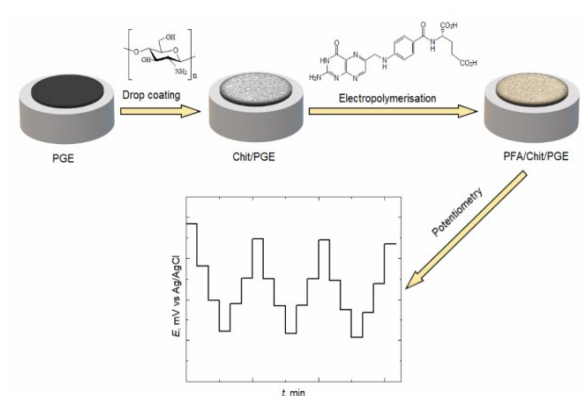
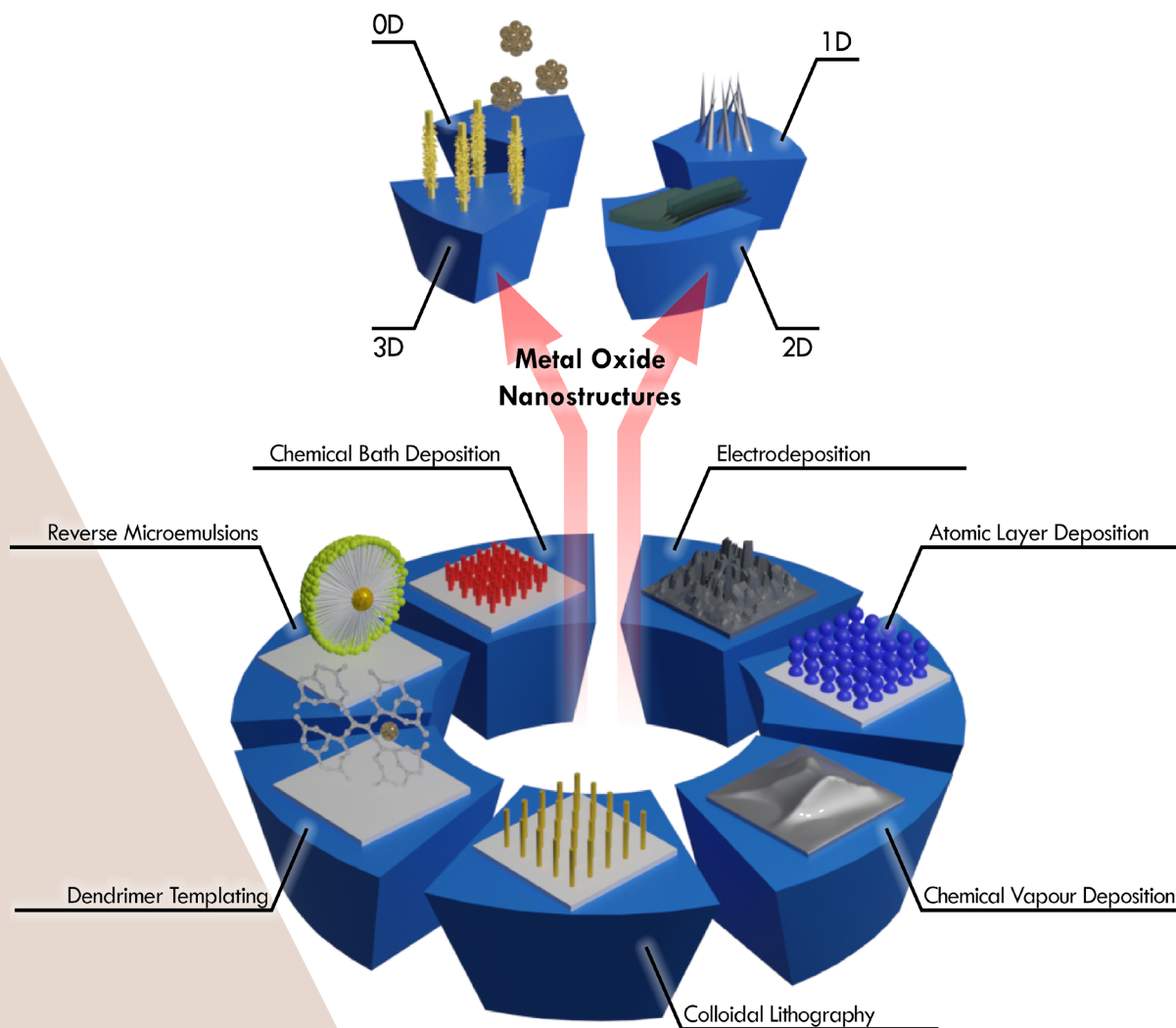


Fig. 2. Scheme of the potentiometric pH sensor development.



# Nanotechnology



## The Department of Nanotechnology

The main research directions the Department of Nanotechnology, established in the beginning of 2022, are dedicated to the development of sensors, biosensors, immuno-analytical systems, molecularly imprinted polymer-based sensors, DNA sensors and other related research topics. Redox-active polymers are currently featured as a promising class of electron mediators. Therefore, a significant part of our experiments focus on development of optical, acoustic and electrochemical sensors based on conducting polymers (including molecularly imprinted polymers) sensitive to SARS-CoV-2 proteins. The optical and acoustic biological sensors are studied by using the methods of spectroscopic ellipsometry and quartz crystal microbalance. The electrochemical sensors based on conducting polymers are studied using differential pulse voltammetry, cyclic voltammetry, pulsed amperometric detection, and some other electrochemical methods.

## Real-time label-free assessment of T7 DNA polymerase immobilization

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Immobilization of DNA-modifying enzymes on any surface is still a complex and challenging task in biotechnology and biosensors. It is very often crucial, especially in biosensors dedicated to the continuous monitoring of DNA. This study is focused on development of continuously operating biosensors based on DNA-modifying enzymes, namely on the real-time monitoring of T7 DNA polymerase immobilization. Quartz crystal microbalance (QCM) was applied for the monitoring of immobilization of T7 DNA polymerase and assessment of analytical signals generated during the action of this enzyme.

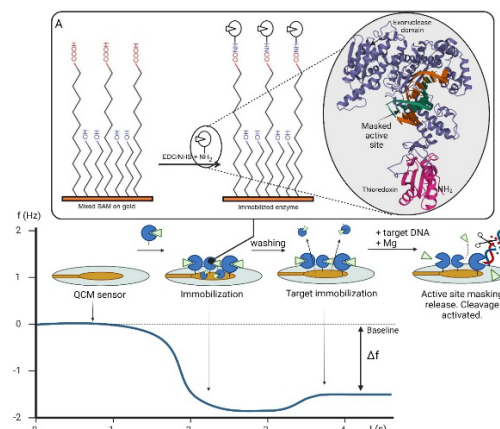


Fig. 1. Scheme of the time-resolved simultaneous measurement of changes in frequency, energy dissipation, and surface saturation of T7 DNA polymerase during the immobilization process on the QCM sensor.

## Comparative study of polydopamine and polypyrrole modified yeast cells applied in biofuel cell design

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Due to high global energy requirements, the research for green-renewable energy has skyrocketed in the past few years. Yeast-based microbial fuel cells (MFCs) could serve as a potential alternative energy source. Redox-active polymers are currently featured as a promising new class of electron mediators with lower cytotoxicity compared to other conventional electron mediators. In this study, we tested two electroconductive polymers, polypyrrole (Ppy) and polydopamine (PDA), which possess good electrical properties and are biocompatible with microorganisms. Both PDA and Ppy modifications are deemed successful, which is indicated by an increase in the charge transfer from the yeast cells to the electrodes. Overall, our

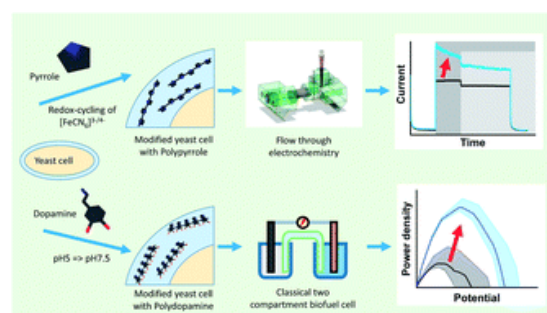


Fig. 2. Scheme of the assessment of polydopamine and polypyrrole-modified yeast cells used in the development of biofuel cells.

modifications applied shorter incubation times in the polymerization bulk solution and generated a greater electric current of approximately a 5-fold power increase compared to the regular yeast MFCs.

## Development of biofuel cells based on anode modified by glucose oxidase, *Spirulina platensis*-based lysate and multi-walled carbon nanotubes

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Bioanode was successfully designed using the chemical oxidized multi-walled carbon nanotubes (CNT) and *Spirulina platensis*-based lysates that facilitate the electron transfer and reduce the open circuit potential (OCP) drop along the electron transfer pathway. Composition, morphology and chemical modification efficiency of CNT was examined using scanning electron microscopy (SEM), energy dispersive X-ray analysis (EDX) and simultaneous thermal analysis (STA) coupled with mass spectrometric (MS) analysis of evolving gaseous species (TG/DTA-MS). The results of this study indicate that glucose oxidase (GOx) immobilized on CNT functionalized with *Spirulina platensis*-based lysates possess superior electron transfer and reduce the OCP drop along the electron transfer pathway (Fig. 3).

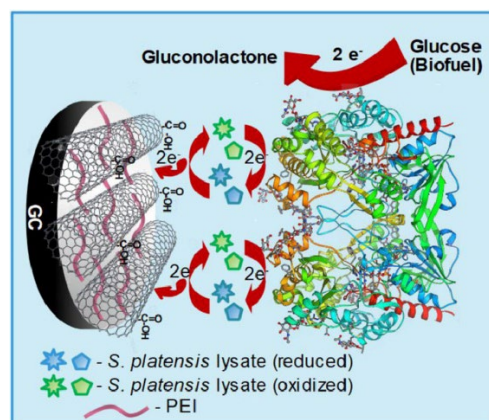


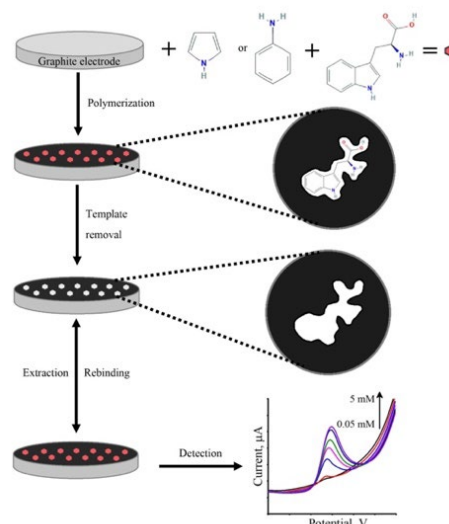
Fig. 3. Scheme of the bioanode consisting of glassy carbon with polyethyleneimine, multi-walled carbon nanotubes and *Spirulina platensis*-based lysates used for the development of biofuel cells.



## Electrochemical sensors based on L-tryptophan molecularly imprinted polypyrrole and polyaniline

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The aim of this work was to compare two different conducting polymers (polypyrrole and polyaniline) in the design of the molecularly imprinted polymer (MIP). An L-tryptophan was selected as a template molecule in such MIP-based layers deposited on the graphite electrodes. Further, the MIPs with L-tryptophan imprints were applied in the design of electrochemical sensors for the detection of L-tryptophan. All polymer layers were electrochemically deposited on the electrode surface by the application of potential cycling. The characteristics of all modified electrodes were evaluated by differential pulse voltammetry (DPV) and cyclic voltammetry (CV). The results demonstrate that the molecularly imprinted polypyrrole MIPpy layer has a greater affinity toward L-tryptophan molecules in comparison with other layers evaluated in this study.



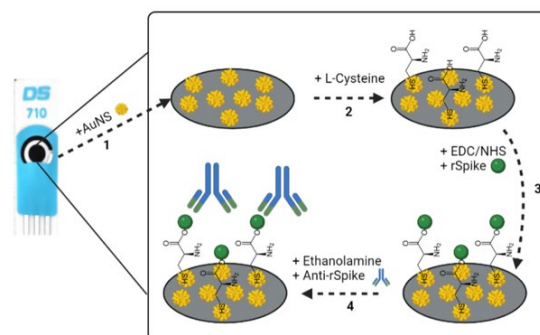
**Fig. 4.** Scheme of evaluation of graphite electrode modified with molecularly imprinted polypyrrole with L-tryptophan imprints. Electrochemical measurements were performed by DPV in 40 mM Britton-Robison buffer solution with 0.1 M of KCl, pH 2.5.

## Determination of rSpike protein by specific antibodies with SPCE modified by electrodeposited gold nanostructures

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The applicability of electrochemical sensing techniques for detecting specific antibodies against severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) spike proteins, in the blood serum of patient samples following coronavirus disease 2019 (COVID-19), was assessed. Herein, screen-printed carbon electrodes (SPCE) with electrodeposited gold nanostructures (AuNS) were modified with L-Cysteine for further covalent immobilization of recombinant SARS-CoV-2 spike proteins (rSpike). The affinity interactions of the rSpike protein with specific antibodies against this protein (anti-rSpike) were assessed using cyclic voltammetry and differential pulse voltammetry methods (Fig. 5).



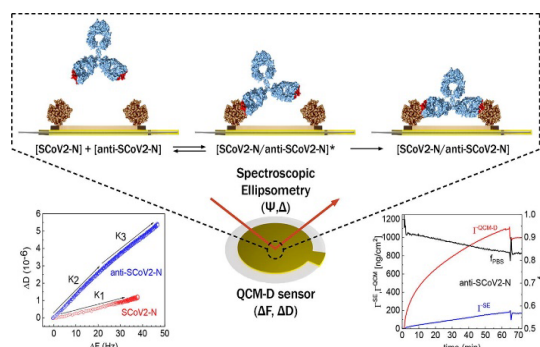
**Fig. 5.** Scheme of experimental stages occurring on the SPCE. (1) The formation of SPCE/AuNS by electrodeposition; (2) SPCE/AuNS/SAM formation; (3) the activation of the SPCE/AuNS/SAM by EDC-NHS mixture following SPCE/AuNS/SAM/rSpike formation; (4) ethanolamine blocking of remaining active functional groups and SPCE/AuNS/SAM/rSpike/anti-rSpike immunocomplex formation via the interaction between immobilized rSpike protein and the anti-rSpike antibodies present in the aliquot.

## Combined SE/QCM-D measurements for assessment of polymer layers and application in biosensing

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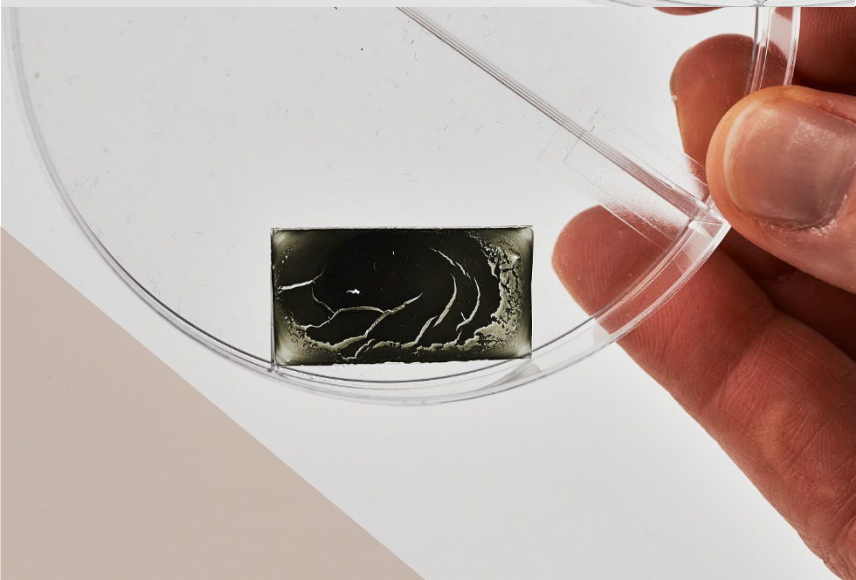
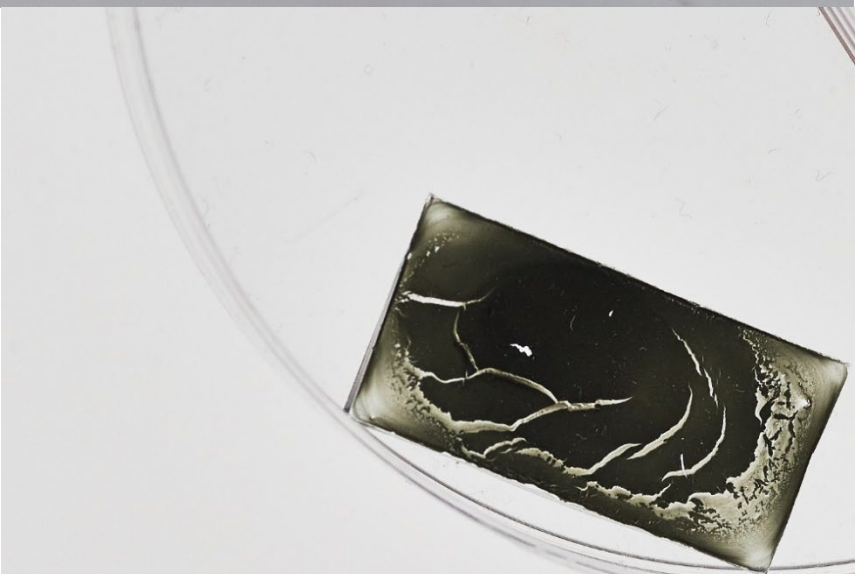
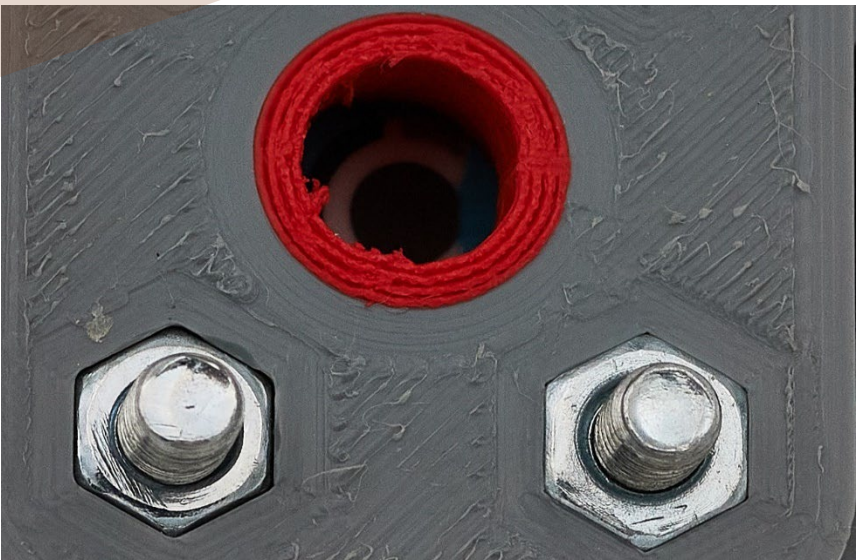
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Detailed evaluation of the antigen and antibody interaction rate and the strength of formed immune complex is very important for medical and bioanalytical applications. These data are crucial for the development of sensitive and fast immunosensors suitable for continuous measurements. Therefore, here the combined spectroscopic ellipsometry and quartz crystal microbalance with dissipation techniques (SE/QCM-D) were used for the evaluation of: (i) covalent immobilization of SARS-CoV-2 nucleocapsid protein (SCoV2-N) on QCM-D sensor disc modified by self-assembled monolayer based on 11-mercaptoundecanoic acid and (ii) interaction of immobilized SCoV2-N with specific polyclonal anti-SCoV2-N antibodies followed by immune complex formation process. The results show that the SCoV2-N monolayer is rigid due to low energy dissipation registered in QCM-D measurement. In contrast, the anti-SCoV2-N layer produced after interaction with the immobilized SCoV2-N formed a soft and



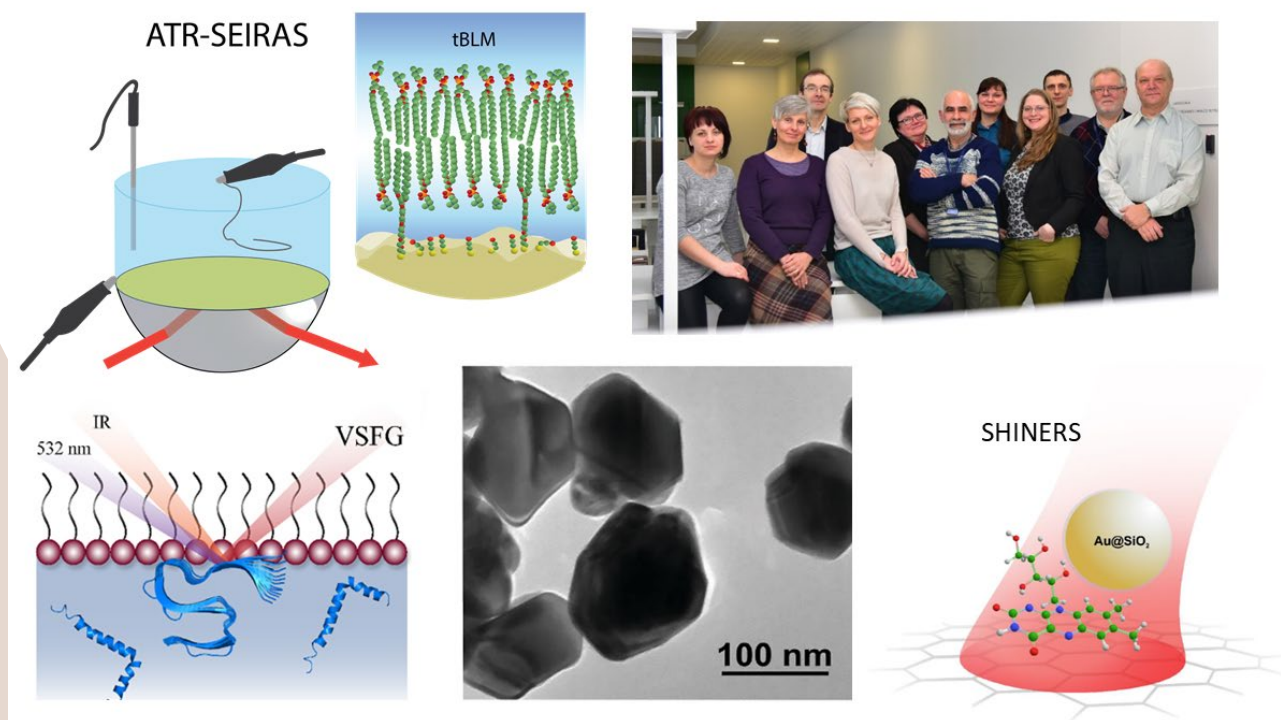
**Fig. 6.** Schematic representation of the anti-SCoV2-N interaction with covalently immobilized SCoV2-N. The immune complex formation is a two-steps process.

viscous layer. Sparse distribution of SCoV2-N on the surface affected the spatial arrangement of the antibody during the formation of immune complexes. The hinge-mediated flexibility of the antibody's Fab fragments allows them to reach more distantly located SCoV2-N and establish a bivalent binding between proteins in SCoV2-N/anti-SCoV2-N complex.





# Spectroelectrochemistry & organic chemistry



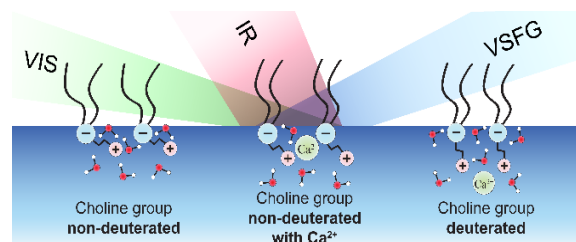
## Spectroscopy for the study of adsorption, electrochemical and biochemical processes at interfaces, organic synthesis and chromatography of environmental objects

The most essential processes in electrochemical catalysis and energy conversion, electrochemical and biochemical electron transfer, as well as biochemical processes occur at surfaces and interfaces. In order to understand and predict these processes, a molecular level understanding is required. In the past few years we attempt to use modern spectroscopy techniques to elucidate how do the molecules adsorb, how do they interact with the surface and each other, how proceed the electron exchange between adsorbate and solution species, as well as other important issues on a molecular level. For these purposes, a number of advanced techniques were elaborated and adopted in our labs, especially those that combine spectroscopy with other complementary techniques like electrochemistry. Among them, Raman spectroscopy, especially some special Raman techniques like Surface Enhanced Raman Scattering (SERS), Resonance Raman Spectroscopy (RRS), as well as their combinations with electrochemical techniques are used. Recently, new Raman technique – Shell-isolated nanoparticle-enhanced Raman Spectroscopy (SHINERS) – was adopted by us to study changes occurring in a molecular structure of self-assembled molecular structures driven by electrochemical potential. Also, graphene-like materials and biological cells were studied by this technique. Vibrational sum-frequency generation (VSFG) spectroscopy was employed for analysis of phospholipids at various deuteration (H/D) levels. Multiwavelength Raman Spectroscopy, as well as its combination with electrochemical techniques were successively applied for the study of electrochemical processes, occurring in electropolymerized layers of conducting polymers. It enables to get a close insight into structural changes occurring in these polymers due to electron transfer. Next to this, organic synthesis on-demand, and chromatographic analysis of various naturally occurring objects like essential oil of plants growing wild in Lithuania are within the scope of our activities.

## Effect of deuteration on a phosphatidylcholine lipid monolayer structure: New insights from vibrational sum-frequency generation spectroscopy

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We have used vibrational sum-frequency generation (VSFG) spectroscopy to elucidate the possible effect of various levels of isotopic substitution (H/D) on the properties of DPPC/D<sub>2</sub>O interface. We found that deuteration of choline group has a great impact on monolayer properties (Fig. 1), while monolayers with deuterated alkyl chains do not exhibit any differences. In addition, deuteration of choline group strongly affects the hydration of the phosphate group.

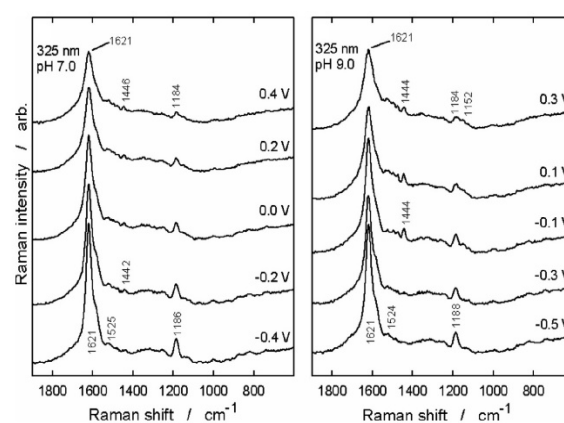


**Fig. 1.** The schematic diagram showing how deuteration of the choline group changes the structure of the lipid's choline group and binding of the Ca<sup>2+</sup> ions.

## Raman spectroelectrochemical study of poly(N-methylaniline) (PNMA) at UV, blue, red, and NIR laser line excitations in solutions of different pH

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A detailed study on Raman spectroelectrochemistry of PNMA layer deposited on a gold electrode was performed. Raman spectra were excited by UV line at 325 nm, a blue line at 442 nm, a red line at 633 nm, and a NIR line at 785 nm in solutions of different pH ranging from 1 to 9, and at different electrode potentials ranging from –0.5 to 0.8 V. UV excitation reveals the features characteristic for the reduced form of PNMA, even within the potential range where the oxidized forms prevail (Fig. 2). Red/NIR excitations result in rich Raman features, disclosing all major redox forms as well as their interconversions by changing of potential. The presence of polaronic form of PNMA even in pH-neutral and alkaline solutions has been disclosed.

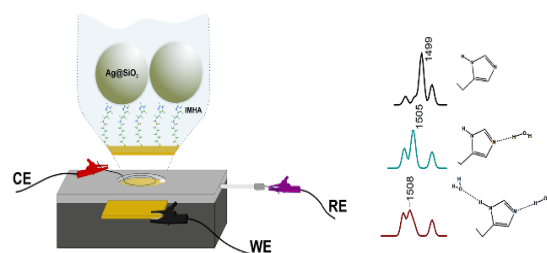


**Fig. 2.** Raman spectra obtained from poly(N-methylaniline) modified gold electrode at 325 nm UV laser line excitation in pH 7.0 and 9.0 solutions at defined electrode potentials.

## SHINERS of imidazole ring functionalized monolayer on smooth gold electrode

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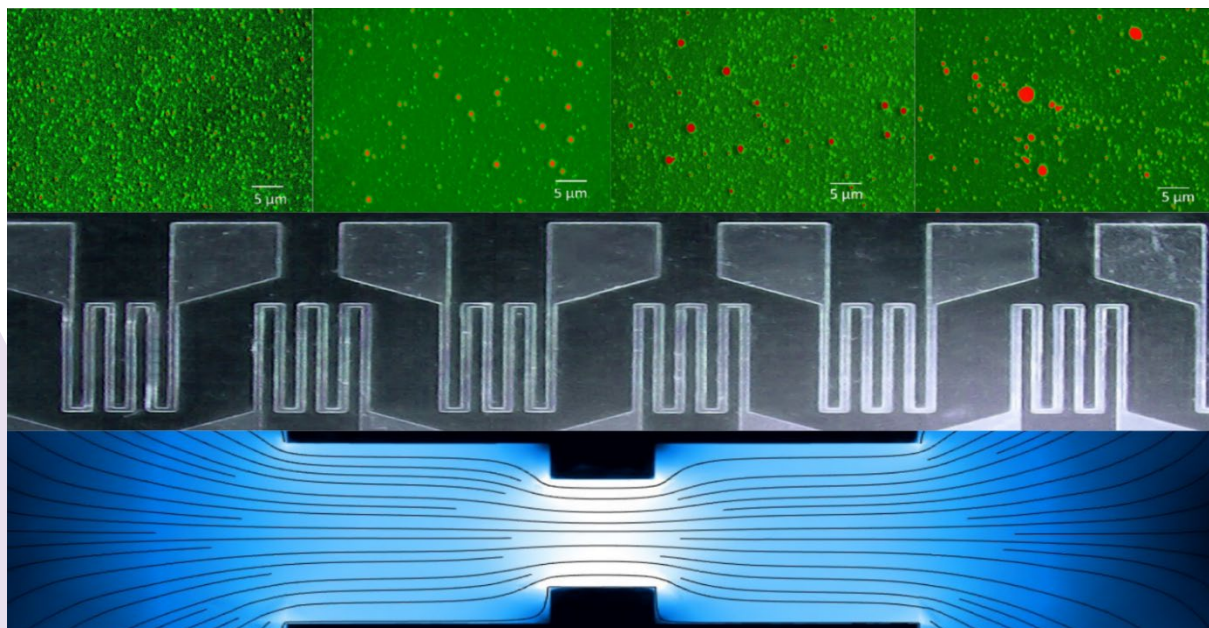
Self-assembled monolayers (SAMs) with functional imidazole (Im) group mimic the histidine side chain at electrified interfaces. In this study, we applied in-situ SHINERS technique to probe the structure of Im-functionalized SAM (Fig. 3). Based on SHINERS study and DFT modeling, the impact of electrode potential on the hydrogen bonding interaction strength of the Im ring was identified.



**Fig. 3.** Scheme of in situ SHINERS experiment and DFT-calculated Raman spectra of model compound (4-ethyl-1-imidazole) with H-bonding coordination number with water molecules from 0 to 2.



# Functional materials & electronics

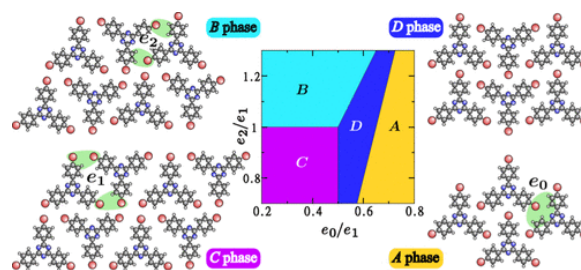


In the last decades, the increasing demand of novel functional materials exhibiting unique properties and used in various applications has led to new discoveries and development of fabrication technologies in this field. In our Department of Functional Materials and Electronics, the technologies of advanced materials, such as thin films and their nanostructures, with tunable properties have been developed and used in various areas of applications. The physical, chemical and biological properties are investigated and combined in developed components and systems. The numerical calculations as well as experimental investigations of inorganic, organic, and biologic structures prepared in our Department are performed using various computational tools and experimental techniques, and responses of these materials to external stimuli (electrical, magnetic, light, microwaves, etc) are studied for wide range of applications.

## Ordering of halogen-functionalized molecules with triazine and benzene core

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Molecular self-assembly via noncovalent interactions is a common approach for directing the synthesis of novel supramolecular networks on solid surfaces. We proposed a model explaining the occurrence of different structures in star-shaped 2,4,6-tris(4-halophenyl)-1,3,5-triazine (TXPT = TBPT, TIPT with X = Br and I) on solid surfaces. The model is universal and could be extended to analogous polyaromatic compounds with benzene core. Density functional calculations reveal that two main interactions of this system have different origins but very similar magnitudes ( $e_1 \approx e_2$ ). This allows the formation of either  $e_1$ -bonded or  $e_2$ -bonded molecular ribbon-like structures. Using our model, we performed the ground-state and the Monte Carlo simulations and finally obtained the phase diagram of the TXPT system, which shows the domains of



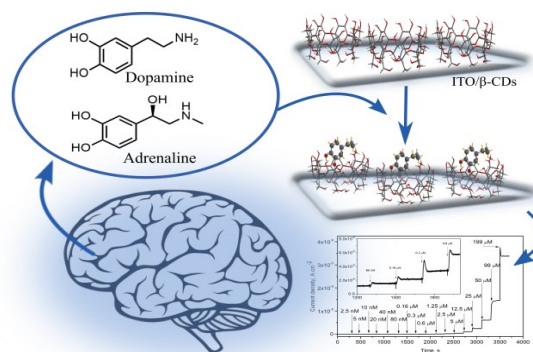
**Fig. 1.** Calculated phase diagram and schematic view of assembled phases. The value  $e_0/e_1 \approx 0.64$  is obtained from density functional calculations.

all four experimentally known structures in a tiny region of the interaction parameters space. The results show that even a slight alteration in the balance of the main interactions leads to the assembly into different supramolecular network. The experimentally known two-phase coexistence is also reproduced in our simulations.

## Self-assembled cyclodextrins-based nanostructures on indium-tin-oxide for a detection of catecholamine neurotransmitters

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Host-guest supramolecular systems are the leading technology to mimic biological systems. The current rapid development of non-enzymatic electrochemical sensors of neurotransmitters shifts the focus towards the host-guest system on electrode that enables to selectively bind these analytes with an electrochemical response. In this study, novel method to deposit  $\beta$ - and  $\gamma$ -cyclodextrin-based self-assembled nanostructures with the sub-nanometer scale size cavities on the indium-tin-oxide glass surface was developed. Our computations demonstrated that neutral and protonated forms of neurotransmitters can be assembled into the cavities and reduce the ionization potential of the analytes. The electrodes with these nanostructures showed the electrochemical response to dopamine and adrenaline as the catecholamine neurotransmitters. The key advantages of the presented electrochemical systems are their simple and cheap preparation, and their ability to achieve the low levels of catecholamine concentration detections.



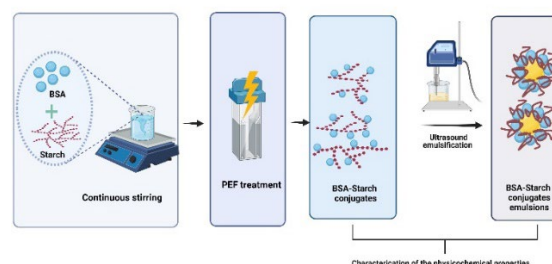
**Fig. 2.** The deposited  $\beta$ - and  $\gamma$ -cyclodextrin-based self-assembled nanostructures with the included analytes and the chronoamperometric detection of dopamine and adrenaline.

## Pulsed electric field-assisted glycation of bovine serum albumin/starch conjugates improved their emulsifying properties

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Applying green technologies in the food industry is critical for sustainable food production. As an eco-friendly food processing approach, pulsed electric field (PEF) has been utilized in food industries to inactivate enzymes and microorganisms without affecting the nutritional quality of treated foodstuffs. Moreover, emulsions are widely applied in the food, drug delivery, and pharmaceutical industries. In our research, PEF could facilitate the Maillard reaction between soluble starch and bovine



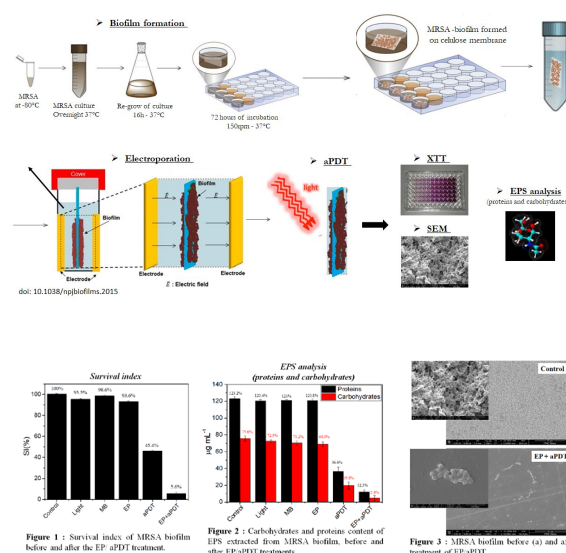
**Fig. 3.** Schematic illustration of PEF application to improve the emulsifying properties of BSA-starch conjugates.

serum albumin (BSA) and improve the emulsifying properties of BSA/soluble starch conjugates. The results of this work could provide fundamental information on the mechanism of PEF-induced Maillard reaction and how PEF can improve the emulsifying properties of the conjugates.

## Effect of electroporation and antimicrobial photodynamic therapy against biofilm matrix of *Staphylococcus aureus*

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Biofilms have been the cause of a wide variety of infections in the human body, reaching 80% of all microbial infections. The bacteria *Staphylococcus aureus* is a leading cause of hospital-acquired infections. The biofilms present specific properties such as the extracellular polymeric substance (EPS), which increases the resistance to antimicrobial treatments. Thus, the development of new approaches is urgent, and antimicrobial photodynamic therapy (aPDT) has been shown as a promising candidate. The aPDT involves the synergistic combination of a photosensitizer (PS), a molecular oxygen and a visible light of appropriate wavelength to produce highly reactive oxygen species (ROS), which leads to the oxidation of several cellular components. Even though this therapy was efficient in attacking many components of the biofilm, the EPS still hampers the PS access to the deeper biofilm cells, promoting the re-grow of the microorganism community. To overcome this problem, the aPDT was combined with electroporation (EP), which affected the EPS contents (proteins and carbohydrates) allowing the PS to reach the biofilm bottom layer and consequently the deeper cells (see Fig. 4).



**Fig. 4.** Top: schematic illustration of aPDT and EP combination to overcome *Staphylococcus aureus*. Bottom: the results obtained using combined aPDT and EP.



## Enhancement of room temperature low-field magnetoresistance in nanostructured lanthanum manganites

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Increasing demand of magnetic field sensors and high-performance magnetometers stimulates rapid advance of various sensors technologies. Technological progress allows to fabricate compact sensors of with enhanced sensitivity, tunable properties and reduced cost for mass production. We demonstrated that the colossal magnetoresistance (CMR) properties of  $\text{La}_{1-x}\text{Sr}_x\text{Mn}_y\text{O}_3$  (LSMO) films grown by pulsed injection MOCVD technique onto  $\text{Al}_2\text{O}_3$  substrate could be tuned by different Sr content ( $0.05 \leq x \leq 0.3$ ) and Mn excess ( $y > 1$ ). We found that the highest values of metal-semiconductor transition temperature  $T_m \sim 270$  K are observed for nanostructured LSMO films with  $x = 0.17 - 0.18$  and  $y = 1.15$ , while the highest low-field magnetoresistance (0.8% at 50 mT) at room temperature ( $\sim 290$  K) was achieved for  $x = 0.3$  and  $y = 1.15$ . The obtained low-field MR values were relatively high in comparison to those for lanthanum manganite films prepared without additional insulating oxide phases. This might be caused by high temperature (383 K), high saturation magnetization at room temperature (870 emu/cm<sup>3</sup>) and relatively thin grain boundaries. The obtained results demonstrate the availability of such materials as CMR sensors for low magnetic field measurements at room temperature.

## Measurement of short pulsed magnetic fields

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Recently, it was demonstrated that high amplitude pulsed magnetic fields could be measured using novel CMR-B-scalar sensors based on the colossal magnetoresistance effect (CMR) of polycrystalline manganites. To measure short magnetic field pulses of microsecond duration, such sensors need to be fast enough with minimized magnetic memory effect. Moreover, the measurement system should be able to record the signal of such a frequency range. Here we propose a magnetic field sensor with minimized magnetic memory effects and meter that compensates electromotive force (EMF) by using the bipolar pulse supply of the CMR-B-scalar sensor. The proposed meter consists of a high-frequency (up to 12.5 MHz) bipolar pulse power generator and 16-bit 25 MS/s differential analogue to digital converter (ADC). The ADC is synchronized with the pulse generator and records the peak-to-peak voltage. The output data of ADC are processed by a microprocessor, which subtracts two neighboring samples (voltage of positive sign and negative sign). As a result, the EMF is eliminated from the measured signal and only the voltage change caused by the magnetic field change is measured. Such a meter can measure high frequency pulsed magnetic fields with pulse duration of several microseconds.

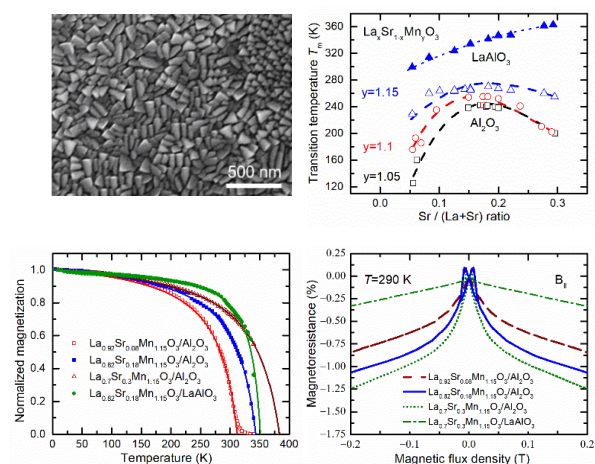


Fig. 5. Top: (left) SEM surface image of LSMO with  $x=0.3$  and  $y=1.15$ , (right)  $T_m$  as a function of Sr content. Bottom: (left) Temperature dependence of magnetization, (right) magnetoresistance as a function of magnetic flux density.

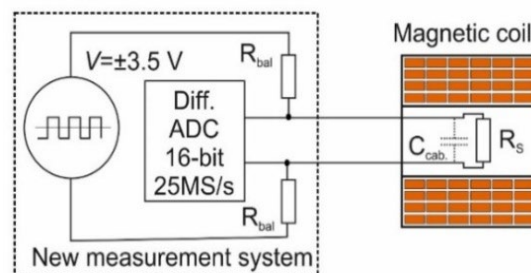


Fig. 6. Block diagram of a measurement system.

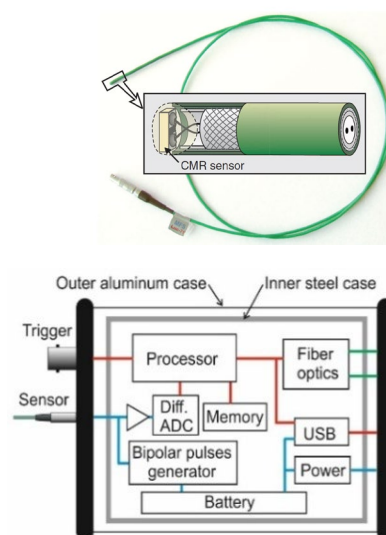
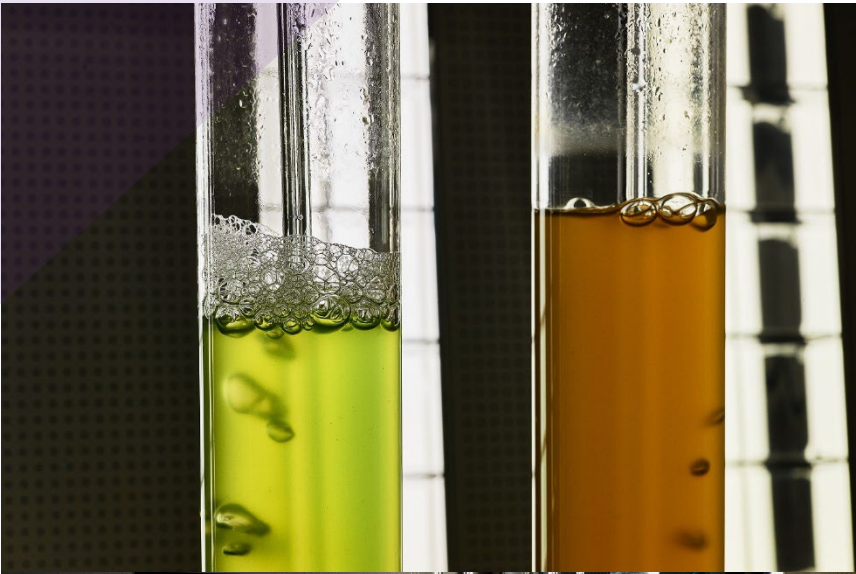
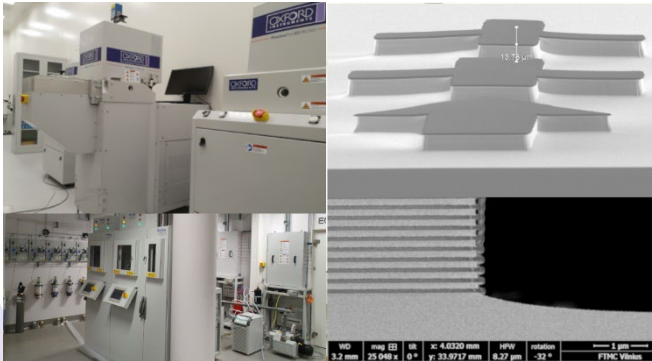


Fig. 7. (Top) Cross-section of CMR sensor. (Bottom) Block diagram of the measure module.





# Nanostructures for applications



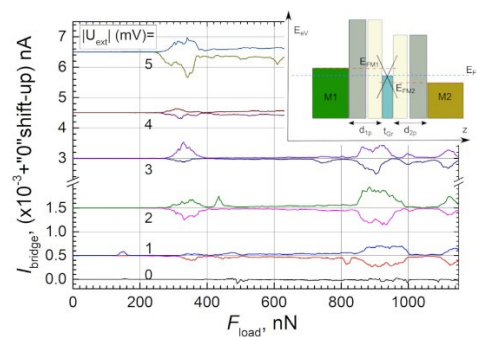
## Hybrid 2D/3D systems for intelligent receptors

Combination of advanced materials and modern technologies creates novel highly attractive approaches in research and development (R&D) of future emerging applied systems with unique properties and innovative functions. Fusion of the electronic and photonic processes in these systems is the fundamental basis for integration of the semiconductor and optoelectronic devices within the hybrid modules acceptable to digitise physical and chemical characteristics. Technology of the hybrid modules allows to develop the key blocks producing the outputs of digital streams with the information about the target objects and processes for the Internet of Things (IoT) and Everything (IoE). In our R&D activities, the semiconductor technology and the system integration methods are improved using advanced knowledge of the modern materials, devices and fundamental processes. Highly attractive ways emerged from the attempts to combine thin films of the usual three-dimensional (3D) materials with the two-dimensional (2D) materials. We are absolutely sure that the 2D/3D hybrid structures can lead to unique working principles of novel devices and new ways for integration of diverse functionalities within a compact autonomous system. We plan to include semiconductor lasers, detectors, photovoltaic-based power sources, and an output signal circuits in these compact systems. Our R&D path to the working prototypes includes three tightly related stages. First, synthesis and investigation of the functional materials and related structures. These studies create the basis for the intentionally controlled technologies of the elements with the two-dimensional (2D) materials in the device fabrication route. There are two classes of the 2D materials, namely graphene and transient metal disulphides (TMDs), that are within the focus of our R&D activities. We found that vertically stacked construction with graphene can combine mechanical, electronic and photonic effects within a multi-parameter receptor acceptable to monitor a complex external influence. Combination of mechanical, electronic, electrical and photonic properties dependent on the van der Waals based integration principles was proved being highly promising because these structures can change the parameters of multi-functional hybrid system in unexpected ways. Second, innovative solutions for prototypes of hybrid devices and their technologies. An exciting way to control the interaction between the electromagnetic waves and the metamaterials was accepted being highly interesting for development of special visualisation systems. There are two primary targets in our scientific and technology studies, namely (i) relationship between the optical – electrical parameters and the core characteristics of the layers and (ii) relationship between the technology conditions and the device parameters. Third, development and testing of the prototypes of the devices and integrated systems. The primary target of this part of the work is to get a solution to the problems that address the needs of potential producers and end-users. For example, development of specific platform for a laser base analyzer was stimulated by successive demonstration of the method acceptable to control the surface coating with polymer materials in an industrial line accomplished by the FTMC team and the private company in the joint project. Based on collaborative efforts, we practically obtained the critical mass of the technology infrastructure required for the high technology level manufacturing of the prototypes of the semiconducting photonic systems. The heading composite picture illustrates the connection between the enabling infrastructure and the produced working structures. This leads to the projects with the technology readiness levels up to the prototypes of devices and pilot technologies.

## Opening and closing of electrical bridges in graphene layer by mechanical force

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It is well known that mono-layer graphene is modified by supporting material so that the in-plane processes can be intentionally controlled. Our results proved that, perpendicular to the plane, the charge transport can predictably be changed by a local compression force. The localized transport bridges can be created across a graphene mono-layer in a metal – graphene – metal (M-G-M) construction in the area with the diameter about 10 – 40 nm. Opening and closing of the bridges depends on the force magnitude as it is illustrated in Fig. 1. Applied external voltage and characteristics of the system are the bridge variables. The bridging is due to the shift in the Fermi level.

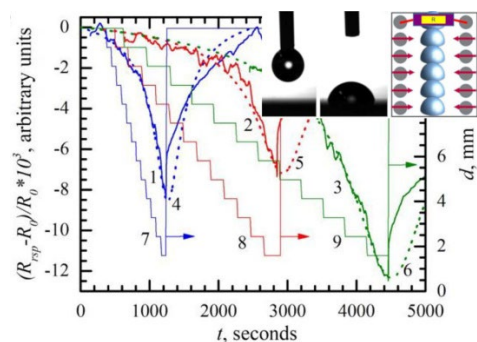


**Fig. 1.** Electrical current perpendicular to the graphene layer measured across the Pt-graphene-Au system as a function of mechanical force  $F_{load}$  for different values of applied external electrical voltage  $U_{ext}$ . Inset: an outline of a band model with the interface barriers outline of a band model with the interface barriers.

## Controlled deposition and applied studies of nano-crystalline graphene

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Unique physical and chemical properties can be investigated in nano-crystalline graphene self-arranged in specific layers during deposition. The results proved that such structures deposited by our technology are acceptable to track the changing position of a water droplet. These structures have the layers with the effective thickness of 0.4–1.1 nm. The position of a water droplet was detected and followed in the air (as in Fig. 2) and on the surface. The time dependences of the electrical resistance of the layers directly correlate with the droplet movement. The response mechanism is due to a hybrid electrical conductance created by a combination of the charge transport of both electrons and mobile ions. This combination depends on the proximity and direct contact of the droplet to the surface.

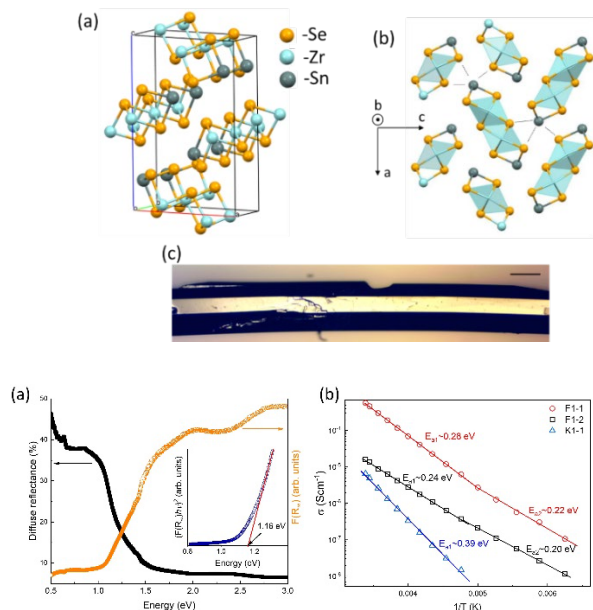


**Fig. 2.** Tracking of water droplet in the space above a layer of the nano-crystalline graphene by the time dependence of the resistance response to the test cycle (droplet appearance at a fixed distance from the layer, approach to the surface and removal from the vicinity) at three rates (blue, red, green) of the approach.

## Synthesis and physical characteristics of narrow bandgap chalcogenide SnZrSe<sub>3</sub>

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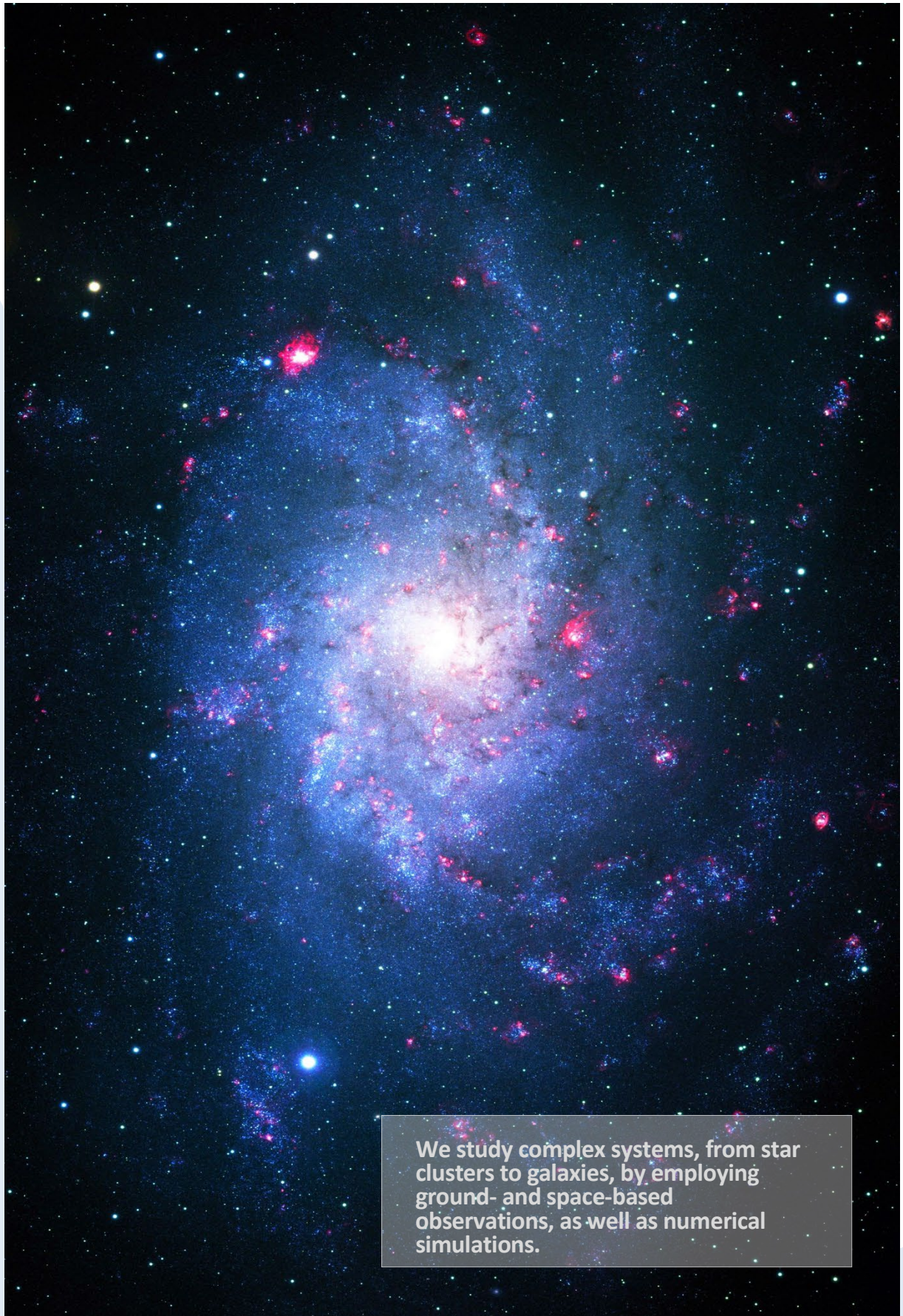
The Sun provides clean and inexhaustible energy which can be harnessed using photovoltaic (PV) technologies. However, manufacture of solar cells uses finite earth resources and depending on the type of technology, it can be energy demanding and emitting large amounts of CO<sub>2</sub>. For these reasons, scientists are constantly improving synthesis and fabrication processes to increase material utilization, upgrading device structure to boost power conversion efficiency and study stability dynamics to prolong PV device lifetime. Here we focus on investigating a compound composed of non-toxic and earth-abundant elements from ABX<sub>3</sub> chalcogenide family materials – SnZrSe<sub>3</sub>. Using a solid-state reaction method, we synthesized SnZrSe<sub>3</sub> crystals and measured their optical and electrical properties. SnZrSe<sub>3</sub> crystallizes into peculiar quasi-one-dimensional (needle-like) structure of double edge sharing ZrSe<sub>6</sub> octahedra (Fig. 3, top). We found that a bandgap of SnZrSe<sub>3</sub> is in a suitable range for application in solar cells (Fig. 3, bottom). Additionally, the electrical measurements indicated that SnZrSe<sub>3</sub> can be engineered to behave as *n*- or *p*-type semiconductor which is very important for formation of semiconductor devices. We believe that SnZrSe<sub>3</sub> is an interesting material candidate for development of more sustainable PV technologies.



**Fig. 3.** Top: (a,b) crystalline structure of SnZrSe<sub>3</sub> at various projections; (c) optical image of SnZrSe<sub>3</sub> crystal. Bottom: (a) absorption coefficient of SnZrSe<sub>3</sub> calculated from diffused reflectance; (b) conductivity as a function of reciprocal temperature demonstrating various activation energies.



# Astrophysics



We study complex systems, from star clusters to galaxies, by employing ground- and space-based observations, as well as numerical simulations.



## Recent star formation history of the dwarf irregular galaxy Leo A

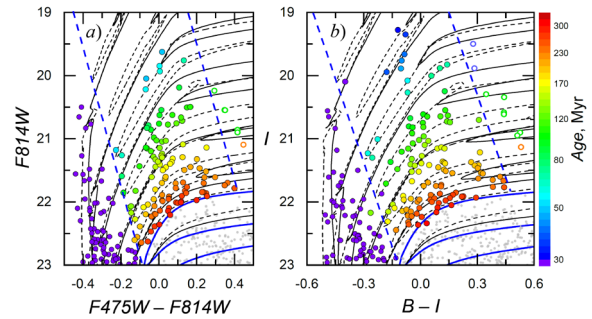
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LeoA is a gas-rich dwarf irregular galaxy of low stellar mass and metallicity. Its star formation history extends up to 10 Gyr. In the present epoch, LeoA is a highly isolated galaxy, which allows for it to be studied in a self-propagating star formation regime. Our aim was to study the star formation history of the Leo A galaxy over the last ~300 Myr. We analysed populations of main sequence (MS) and blue helium-burning (BHeB) stars using multi-colour photometry data obtained with the Subaru Suprime-Cam and the Hubble Space Telescope (HST) ACS cameras. We made use of colour-magnitude diagrams and stellar isochrones to determine individual ages of the BHeB stars, which enabled us to study the evolution of spatial distributions of these stars. We also studied a well-known HI hole in the LeoA galaxy and found that there is a prominent difference in the surface number density of stars in the western and eastern parts of the hole. The bright young (<20 Myr) MS stars residing in the western part of the hole indicate the recent star-forming activity in this region after the quiescent period of ~300 Myr. Furthermore, there is a shock front that closely resembles the shape of the western edge of the HI hole. This shock front could have been formed by the combined stellar feedback from the young MS stars or a Type II supernova located within the HI hole.

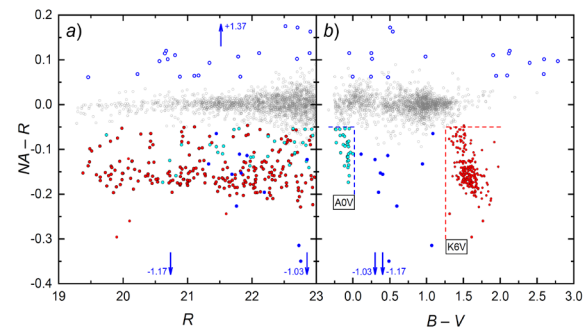
## Dwarf irregular galaxy Leo A. Suprime-cam stellar photometry

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We have surveyed a complete extent of Leo A, which is an apparently isolated Local Group dwarf irregular galaxy, in  $BVR/I + NA$  (centered on  $H\alpha$ ) passbands with the Subaru Telescope equipped with the Suprime-Cam mosaic camera. Photometry results of more than 25000 objects in the field of  $20 \times 24$  arcmin are presented. The catalogue could serve for future imaging and spectroscopic observation programs of Leo A. Also, we have developed an effective method to separate Milky Way (MW) M-type dwarfs and late-type evolved stars in external galaxies by using  $BVR + NA$  passbands.



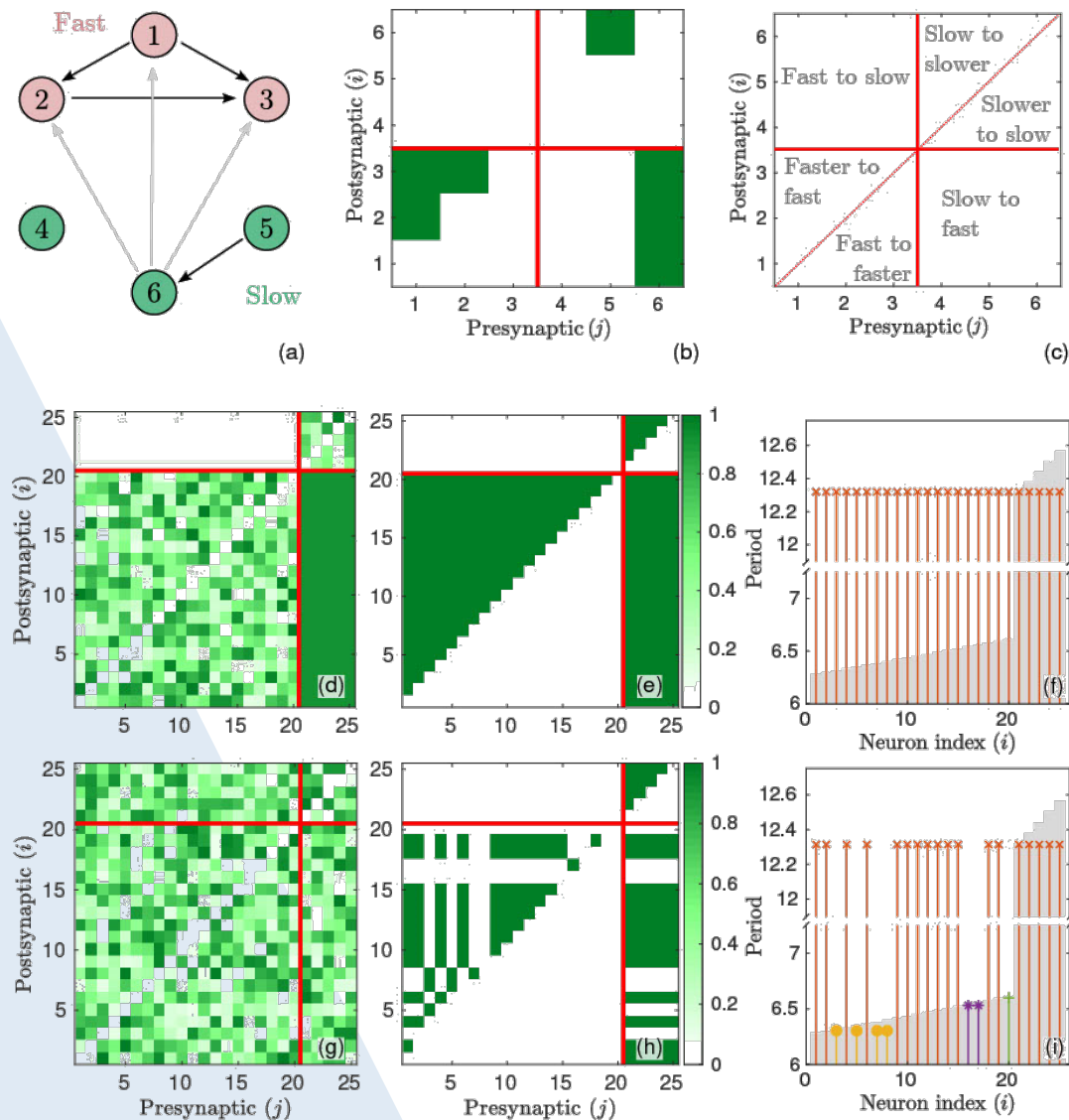
**Fig. 1.** A new method to derive star formation histories in resolved galaxies was proposed. Panels show: (a) HST and (b) Subaru telescope data. The two parallel blue dashed lines confine BHeB stars (colour-coded by age) for which individual ages were determined. Main sequence stars are marked by violet dots. The isochrones of the ages from 15 to 320 Myr are plotted for reference.



**Fig. 2.** The bright ( $R < 23$ ) star-like objects in the Leo A field are plotted as grey dots. Two groups of stars with flux excesses ( $NA-R < -0.05$ ) in the  $NA$  passband are overplotted: MW late-type stars (red dots) and the Leo A early-type emission-line stars (cyan dots). Blue dots mark objects with a significant flux excess in the  $NA$  passband which do not belong to the previous two groups of stars (red and cyan dots). Blue open circles mark stars with a significant flux deficit in the  $NA$  passband. Blue arrows mark objects beyond the limits of figure; numbers adjacent to arrows indicate values of their  $NA-R$  color index.



# Nonlinear dynamics and neuroscience



**Fig. 1.** Examples of connectivity patterns emerging in plastic networks of quadratic integrate-and-fire (QIF) neurons. (a)-(c) A network of six neurons, the first three of which are fast and the next three are slow. (a) Network configurations in the post-transient regime. The arrows indicate the direction of the connections. (b) Asymptotic values of the elements of the connectivity matrix shown in color. This matrix corresponds to the network configuration depicted in (a). Panel (c) explains the structure of connections in the connectivity matrix. Red vertical and horizontal lines separate the regions of slow and fast neurons. (d)-(i) Two examples of the initial and asymptotic states of a network consisting of 20 fast and 5 slow neurons. (d) Initial values of the connectivity matrix with partially random and partially deterministic choice of elements. (e) The asymptotic values of the connectivity matrix obtained from the initial matrix shown in (d). (f) The distribution of natural (grey bars) and actual (vertical red lines ending in crosses) periods of neurons in the post-transient regime. (g) The initial connectivity matrix with all elements chosen randomly. (h) and (i) Same as (e) and (f) but for the initial matrix shown in (g).

We apply methods of nonlinear dynamics and control theory to analyze and control various dynamic modes in large neural networks. In the thermodynamic limit, the network of synaptically coupled quadratic integrate-and-fire (QIF) neurons can be reduced to an exact low-dimensional system of mean-field equations. This makes it possible to carry out a detailed bifurcation analysis of such systems and find regions in the parameter space where collective synchronized oscillations occur. Pathologically excessive synchronization in neural networks is commonly associated with various neurological diseases such as Parkinson's disease. Mean field equations are useful not only to better understand the mechanism of neural synchronization, but also to develop and test various neurostimulation techniques to suppress unwanted synchronization.

## Interplay of different synchronization modes and synaptic plasticity in a system of class I neurons

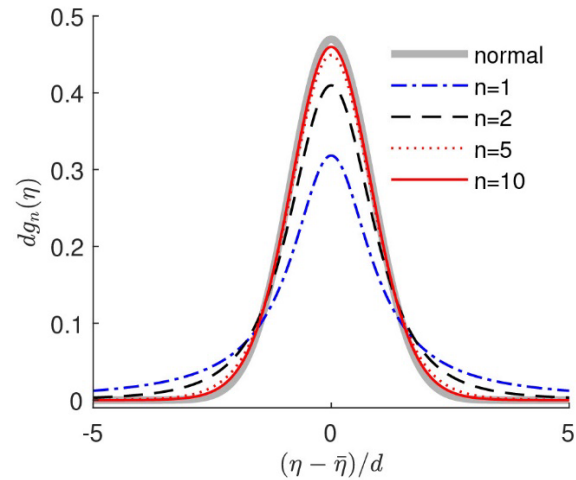
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We analyze the effect of spike-timing-dependent plasticity (STDP) on a system of pulse-coupled class I neurons. STDP is a phenomenon in which the precise timing of spikes affects the sign and magnitude of changes in synaptic strength. STDP plays a crucial role in memory formation and maintenance. Our research begins with a system of two mutually connected QIF neurons, which are canonical representatives of class I neurons. Class I neurons generally have a purely positive phase response curve, indicating that perturbations always produce an advance of their phase. Along with various asymptotic modes previously observed in other neuronal models with plastic synapses, we found a new stable synchronous mode characterized by unidirectional link from a slower neuron to a faster neuron. In this frequency-locked mode, the faster neuron emits multiple spikes per cycle of the slower neuron. We analytically obtain the Arnold tongues for this mode without STDP and with STDP. We also consider larger plastic networks of QIF neurons and show that the detected mode can manifest itself in such a way that slow neurons become pacemakers (see Fig. 1).

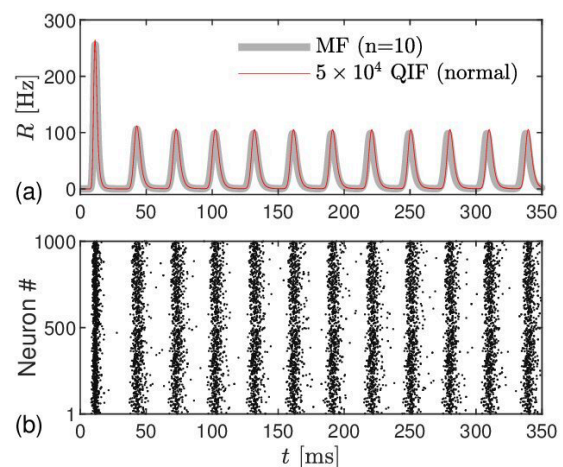
## Mean-field equations for neural populations with $q$ -Gaussian heterogeneities

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Describing the collective dynamics of large neural populations using low-dimensional models for averaged variables has long been an attractive task in theoretical neuroscience. Recently developed reduction methods make it possible to derive such models directly from the microscopic dynamics of individual neurons. To simplify the reduction, the Cauchy distribution is usually assumed for heterogeneous network parameters. Here we extend the reduction method for a wider class of heterogeneities defined by the  $q$ -Gaussian distribution. The shape of this distribution depends on the Tsallis index  $q$  and gradually changes from the Cauchy distribution to the normal Gaussian distribution as this index changes (Fig. 2). We derive the mean-field equations for an inhibitory network of QIF neurons with a  $q$ -Gaussian distributed excitability parameter. It is shown that the dynamic modes of the network significantly depend on the form of the distribution determined by the Tsallis index. The results obtained from the mean-field equations agree well with the results of numerical simulation of the microscopic dynamics of a large network consisting of  $5 \times 10^4$  neurons (Fig. 3).



**Fig. 2.** The  $q$ -Gaussian distribution for different values of the modified (integer) Tsallis index  $n$ . For  $n=1$ , the  $q$ -Gaussian distribution coincides with the Cauchy distribution (blue dash-dotted curve), and for  $n$  going to infinity with the normal Gaussian distribution (thick grey curve).



**Fig. 3.** Dynamics of a population of normally distributed  $5 \times 10^4$  neurons and its approximation by mean-field equations. (a) Firing rate obtained from the microscopic model (thin red curve) with the normal distribution and from the mean-field equations (thick grey curve) with the  $q$ -Gaussian distribution at  $n=10$ . (b) Raster plot of 1000 randomly selected neurons. The dots show the spike moments for each neuron, where the vertical axis indicates neuron numbers.



## Skyrmionic properties of the spherically polarized Bessel beam

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A different type of Bessel-like vortex beam was investigated with its intensity spherically modified by a point-like polarization singularity. Conventional vector Bessel-Gaussian beams are either linearly or radially (and azimuthally) polarized and their transverse structure is preserved under propagation. Here, the Bessel-like beams with a Gaussian envelope are spherically polarized: the electric fields are oriented along the radius vector or along a combination of meridional and azimuthal vectors. The intensity distribution of the beam can be controlled by a proper choice of parameters such as the cone angles of individual plane-wave components and sizes of Gaussian apertures. Moreover, the polarization singularity has a particle-like topology, which can be identified as an optical skyrmion, whose properties were studied (Fig. 4).

## Investigation of the Pancharatnam–Berry phase element for the generation of the top-hat beam

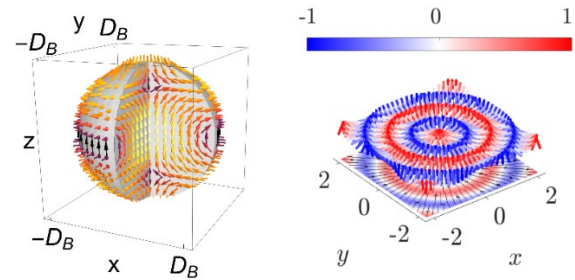
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Within optics, the Pancharatnam–Berry phase (PBP) enables the design and creation of various flat special optical elements such as top-hat converters. We present a study on engineering efficient vectorial top-hat converters inscribed in glass by high-power femtosecond laser pulses. We phase encode a top-hat converter and demonstrate how its quality is influenced by various parameters. We theoretically investigate the top-hat beam's generation under imperfect conditions such as the mismatch of the incident beam width or the misalignment of the center of the converter. Experimental verification of the concept is also presented.

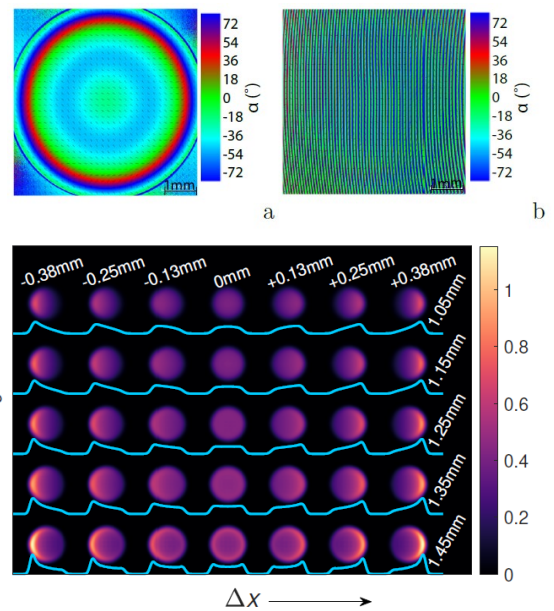
## Azimuthally and radially polarized pulsed Bessel-X vortices

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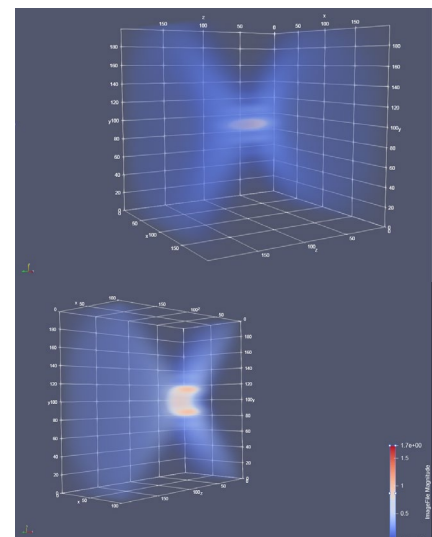
Invariant wave packets receive ever-increasing research attention due to their unique and useful properties, such as diffraction resistance, nondispersive propagation, self-healing, and others. These abilities become even more interesting when combined with optical vorticity, short pulse durations, high powers, and inhomogeneous polarization. This work presents an analytical model of pulsed fields, invariant to propagation, with both optical vorticity and radial/azimuthal polarization. We investigated the structure of electromagnetic fields, their propagation properties for different cone angles, and the duration of Bessel-X pulses (see Fig. 6).



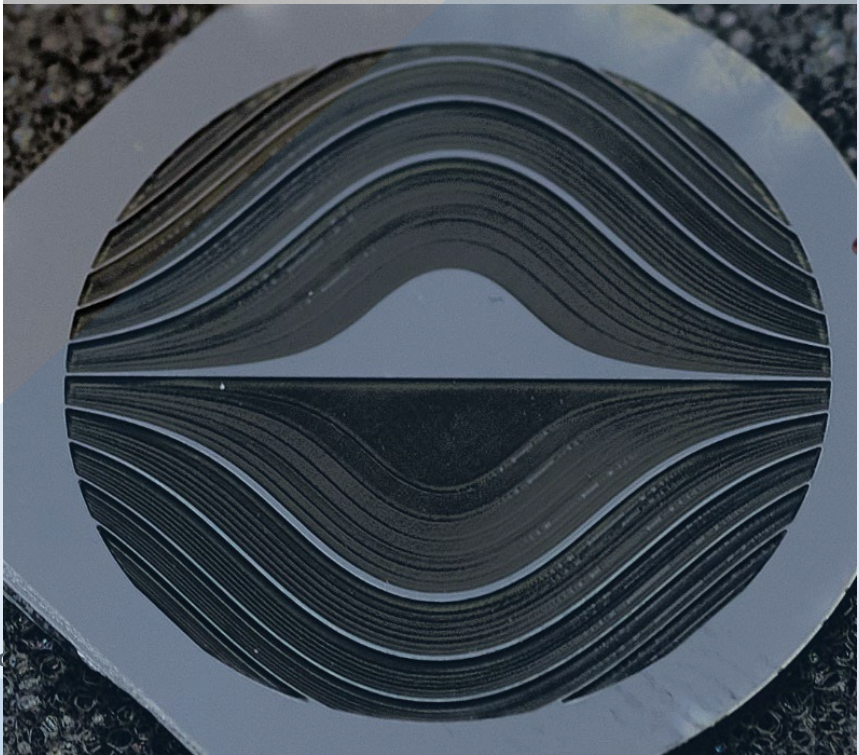
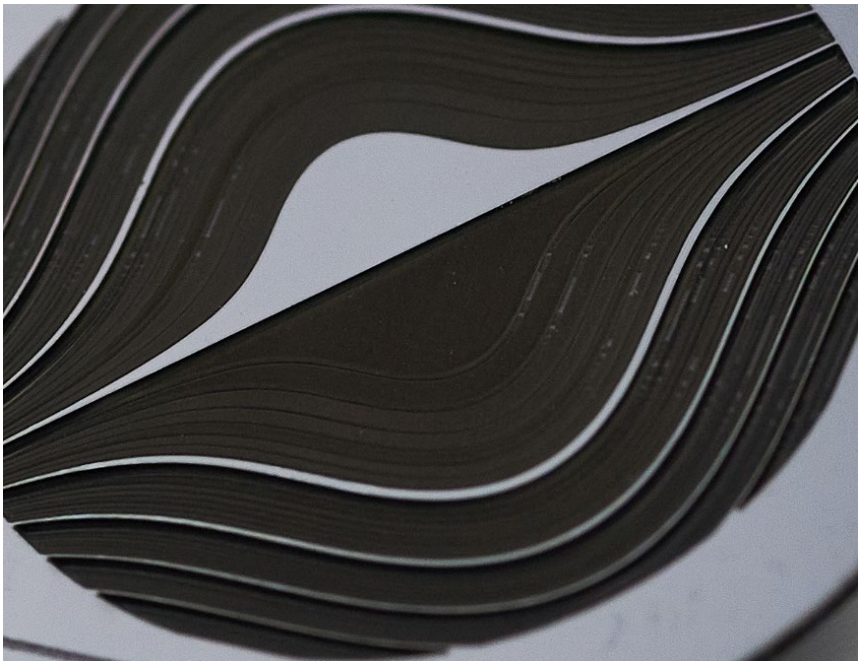
**Fig. 4.** (a) Schematic representation of the electric field orientations in transverse electric spherically polarized Bessel vortex with topological charge  $m = 0$ . (b) Skyrmionic charge and schematic representation of the skyrmion at  $z = 0.85 z_0$ . The angle of the Bessel beam is  $45^\circ$ .



**Fig. 5.** Experimentally obtained slow axis angle distribution of the two manufactured PBP elements. The PBP element is (a) without and (b) with the blazed grating,  $\gamma = 1.6^\circ/\mu\text{m}$ . (c) The transverse intensity distribution of beams produced by the PBP element at the distance  $z = z_0$  for various displacements of the PBP element  $\Delta x$  (horizontally) and sizes of the incoming Gaussian beam  $d_0$  (vertically).

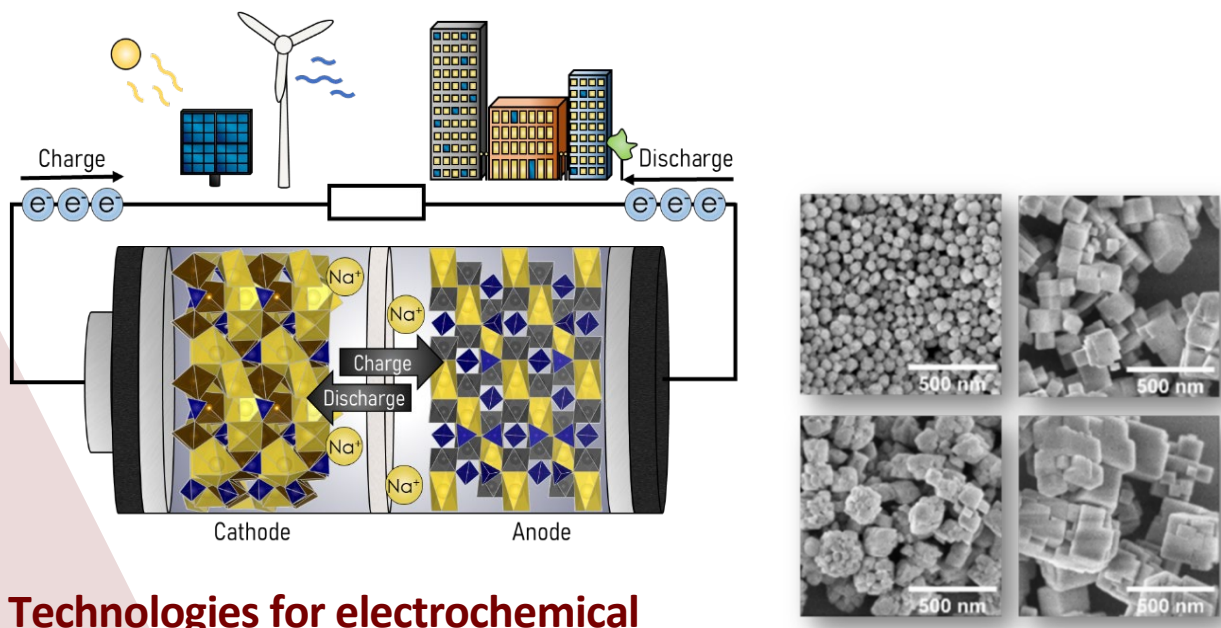


**Fig. 6.** Three-dimensional intensity distribution of a linearly polarized optical vortical X-pulse with topological charge  $m=0$  (on the top) and  $m=2$  (on the bottom). The cone angle is 45 degrees, and the normalized spectral width is 0.2.





# Electrochemical material science



## Technologies for electrochemical energy conversion and storage, solar-driven electrochemistry and smart coatings

The search and development of novel energy storage solutions is recognized as one of the key tasks in modern science. Electrochemical energy conversion and storage technologies offer attractive solutions for many current renewable energies related problems. The R&D activities in this area in Departments of Electrochemical Material Science and Chemical Engineering and Technology are focused on the development and profound understanding of materials, processes and devices for safe, sustainable and low-cost aqueous Na-ion batteries for stationary energy storage applications (NaAquaCell project), photoelectrochemical production of hydrogen and strong oxidants suitable for water treatment (CatWatSplit project), electrochemical synthesis of silicon nanostructures and other materials, including superparamagnetic and luminescent nanoparticles with possible applications in photovoltaics, nanomedicine, etc. Electrochemical, chemical as well as physical methods (electrodeposition, atomic layer deposition, magnetron sputtering) are applied for the surface modification and production of smart materials with exceptional electrocatalytic, anticorrosive, magnetic, mechanical or other properties. The integral part of the process of new materials development is a thorough characterization of their structure, morphology and chemical composition. Environmental friendliness and sustainability are imperative for all newly developed technologies.

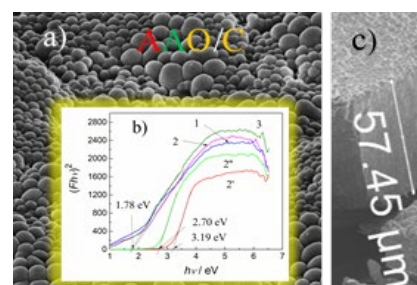
Extended experience in electrochemistry and material science is the main driving force in developing innovative sustainable technologies and new applications for circular economy. Anodic coatings on aluminum, fortified by depositing nanoscale layers of selected metals and oxides, show very promising tribological characteristics and good biocompatibility. Major focus has also been devoted to the diffusion of organic compounds, such as corrosion inhibitors, antiwear additives, colorants or adhesives, into electrochemically nanostructured coatings. Significant attention has been paid to the properties of natural deep eutectic solvents, which are very promising industrially. These solvents are investigated in great detail during the H2020 project TERMINUS. A critical task of this project, tackled by FTMC Tribology laboratory, targets the development of adhesives for recyclable multilayer packaging.

Smart coatings with active corrosion protection ability for metals in aggressive environments are developed. Corrosion tests are carried out in the Accredited Corrosion Research Laboratory at FTMC, which performs characterization and evaluation of the corrosion-caused changes in metals, alloys, composite coatings, paints and lacquers in natural and artificial atmospheres and can also assess the microbially induced corrosion of materials in ambient atmosphere or model media.

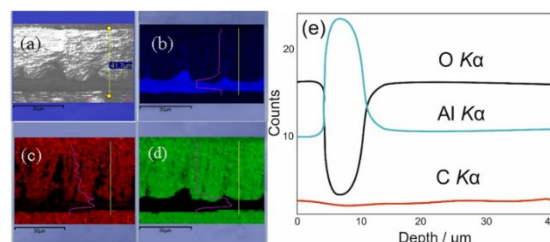
## Designing carbon enriched alumina films possessing a visible light absorption

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Fabrication of hybrid-type metal oxide films with entrapped carbonaceous species is one of our priority tasks. Here we report on the possibility to form the thick aluminum anodic oxide (AAO) films hybridized with a surprisingly high content of entrapped carbonaceous species. We designed a one-step process of Al anodizing in an aqueous slightly acidic solution containing  $\text{NaVO}_3$  and formic acid at an ambient temperature and a constant bath voltage of 60 to 100 V. This regime is much simpler than high-field burning anodization of Al reported for other organic acid electrolytes. The obtained films were characterized by scanning electron microscopy, X-ray photoelectron spectroscopy, X-ray Auger electron spectroscopy, thermogravimetry analysis, ellipsometry, and energy dispersive X-ray spectroscopy. We also analyzed diffuse reflection and transmission spectra. The absorption edge of a visible light ( $\sim 1.78$  eV) was found and explained by entrapment of vanadium ions and carbonaceous species. Possible application of porous alumina films with a high amount of entrapped carbon and graphene in future technologies looks promising.



**Fig. 1.** Typical (a) back side and (c) and cross-sectional SEM images of porous AAO/C film. In (b): Tauc plots for direct transitions in the AAO/C films fabricated by Al anodizing in 0.2  $\text{NaVO}_3$  and 0.8 M  $\text{HCOOH}$  solution at 60 (1); 80 (2), and 100 V (3) for 1 h and at 80 V for 2 (4) and 5 min (5).

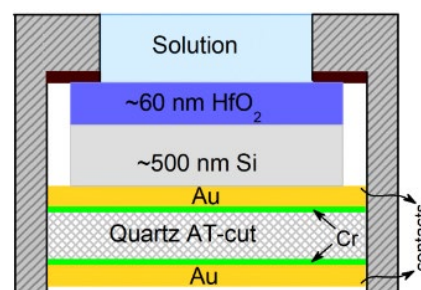


**Fig. 2.** (a) Cross-sectional image of AAO/C composite film and EDS mapping of (b) aluminum, (c) carbon and (d) oxygen elements. (e) Cross-sectional distribution curves of oxygen, aluminum and carbon elements in the film.

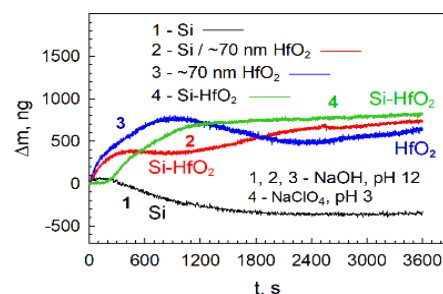
## Silicon passivation by ultrathin hafnium oxide layer for photoelectrochemical applications

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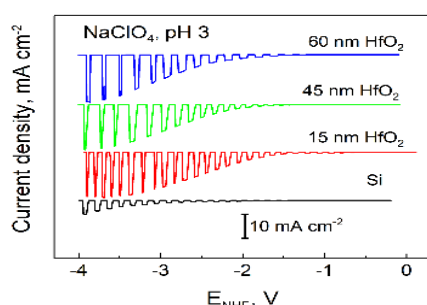
Hafnium oxide ( $\text{HfO}_2$ ) films on silicon have the potential for application in photovoltaic devices. In this study, ultrathin films of  $\text{HfO}_2$  in the range of 15–70 nm were deposited on p-Si and Au substrates by atomic layer deposition. Quartz crystal nanogravimetry with Si and Au substrates indicated dynamics of electrolyte intake into the oxide film. Mott–Schottky plots showed that the dark Si surface adjacent to the  $\text{SiHfO}_2$  interface is positively charged in an acid electrolyte. The number of photoelectrons was determined to be much greater than the doping level of silicon. The cathodic photoactivity of the p-Si electrode protected by  $\text{HfO}_2$  films was studied with respect to the reaction of hydrogen reduction in acid solution. In acid solution, the film enhanced the reduction process when compared to that on the coating free electrode. The acceleration effect was explained in terms of prevention of silicon oxide formation, whose passivating capability is higher than that of hafnia films. Hafnia films protected Si from corrosion in this medium; however, at the same time, the film reduced electrode activity.



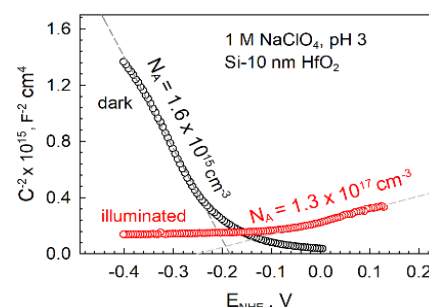
**Fig. 3.** Principal configuration of the QCN sensor.



**Fig. 4.** Mass change determined by the QCN.



**Fig. 5.** Cathodic photocurrents of hydrogen reduction over wide region of cathodic voltages.



**Fig. 6.** Mott–Schottky plots for p-Si with 10-nm  $\text{HfO}_2$  layer in the dark and under illumination ( $\lambda=505$  nm).



## Electrochemical characterization of NASICON-type $\text{Na}_{3-x}\text{V}_{2-x}\text{Ti}_x(\text{PO}_4)_3$ ( $0.0 < x < 1.0$ ) as aqueous Na-ion battery positive electrodes

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Phosphate frameworks with NASICON structure are among the most studied and applied Li- and Na-ion battery electrode materials. In this work, the NASICON-structured  $\text{Na}_{3-x}\text{V}_{2-x}\text{Ti}_x(\text{PO}_4)_3$  with  $x = 0.0, 0.25, 0.5, 0.75$  and  $1.0$  were successfully prepared by conventional solid-state synthesis and characterized in detail as potential aqueous Na-ion battery positive electrodes with improved charge capacity and cycling stability. Structural analysis using powder X-ray diffractometry indicates that Ti substitutes V at arbitrary concentration without significant distortion of the NASICON structure. The results show that Ti content in this system directly correlates with its aqueous stability in 1 M  $\text{Na}_2\text{SO}_4$  aqueous electrolyte. Electrochemical kinetics and charge capacity measurements show  $\text{Na}_2\text{VTi}(\text{PO}_4)_3$  as well as  $\text{Na}_{2.25}\text{V}_{1.25}\text{Ti}_{0.75}(\text{PO}_4)_3$  to be stable positive electrodes in simple aqueous electrolyte solutions. Hybrid density functional theory analysis of V-O chemical bonding suggests that it is stabilized by the presence of titanium in the NASICON structure. In this work, we show that the observed capacity loss in full symmetric cells is caused by the capacity imbalance between positive and negative electrodes which progresses during cycling but not due to the aqueous material stability *per se*. This imbalance is caused by several parasitic reactions, the most important being oxygen reduction reaction catalyzed by  $\text{Ti}(\text{III})$  species. Careful mitigation and management of this reaction could, in principle, allow the preparation of truly capacity balanced cells (i.e. without a need of any electrode overcapacity), and superior cycling stability.

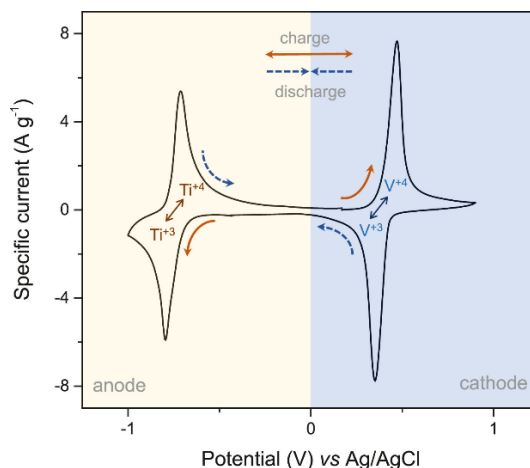


Fig. 7. Schematic representation of anode and cathode reactions occurring in symmetric full-cells with NVTP electrodes during charging and discharging.

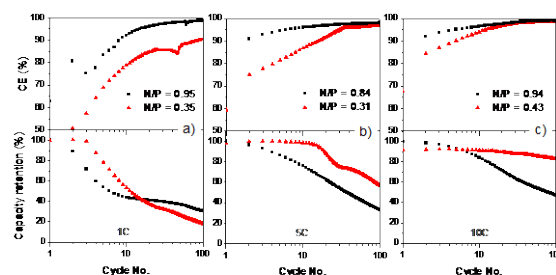


Fig. 8. Galvanostatic charge-discharge cycling data for aqueous symmetric NVTP|NVTP coin cells with different anode/cathode (N/P) capacity ratio and C-rate.

## Influence of morphology on photoanodic behaviour of $\text{WO}_3$ films in chloride and sulphate electrolytes

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Photoelectrochemical (PEC) synthesis is gaining an increasing interest amongst the advanced oxidation processes, which can convert solar energy to chemical energy in the form of value-added oxidants suitable for water treatment and disinfection. To ensure the efficient generation of desired product, careful engineering of semiconductor/electrolyte interface is required. In this study the effect of surface morphology on the competition between the photoanodic oxidation of water molecules and anions occurring on the surface of tungsten (VI) oxide electrodes in sulphate and chloride electrolytes is investigated. Possible photoanodic processes are analysed on the basis of the proposed potential-assisted photochemical approach, which takes into consideration high oxidizing power of photogenerated holes in  $\text{WO}_3$  and formation of radicals as intermediates. Significant role of specific adsorption of chloride ions as well as intermediate products of their oxidation ( $\text{Cl}^\cdot$ ,  $\text{Cl}_2^{\cdot-}$ ) in lowering the photocurrent onset potential, trapping the photogenerated charge carriers as well as protecting  $\text{WO}_3$  surface from accumulation of peroxo species is revealed.

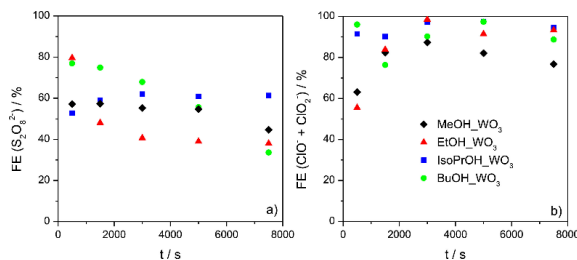
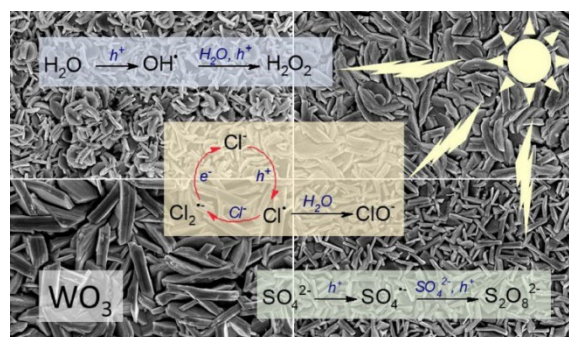
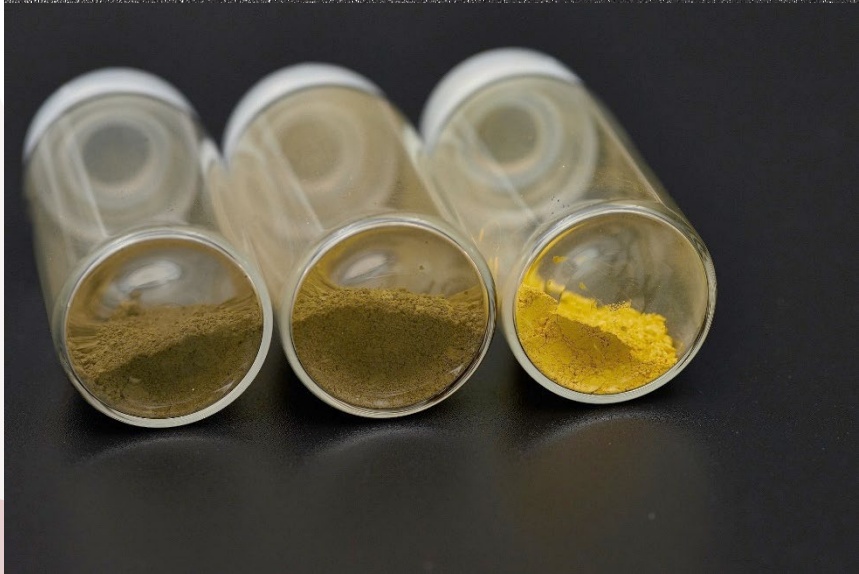
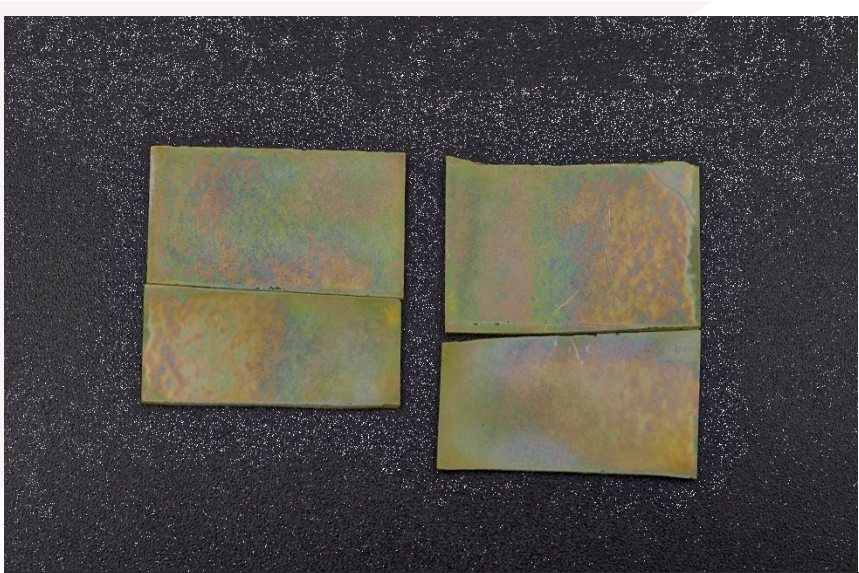
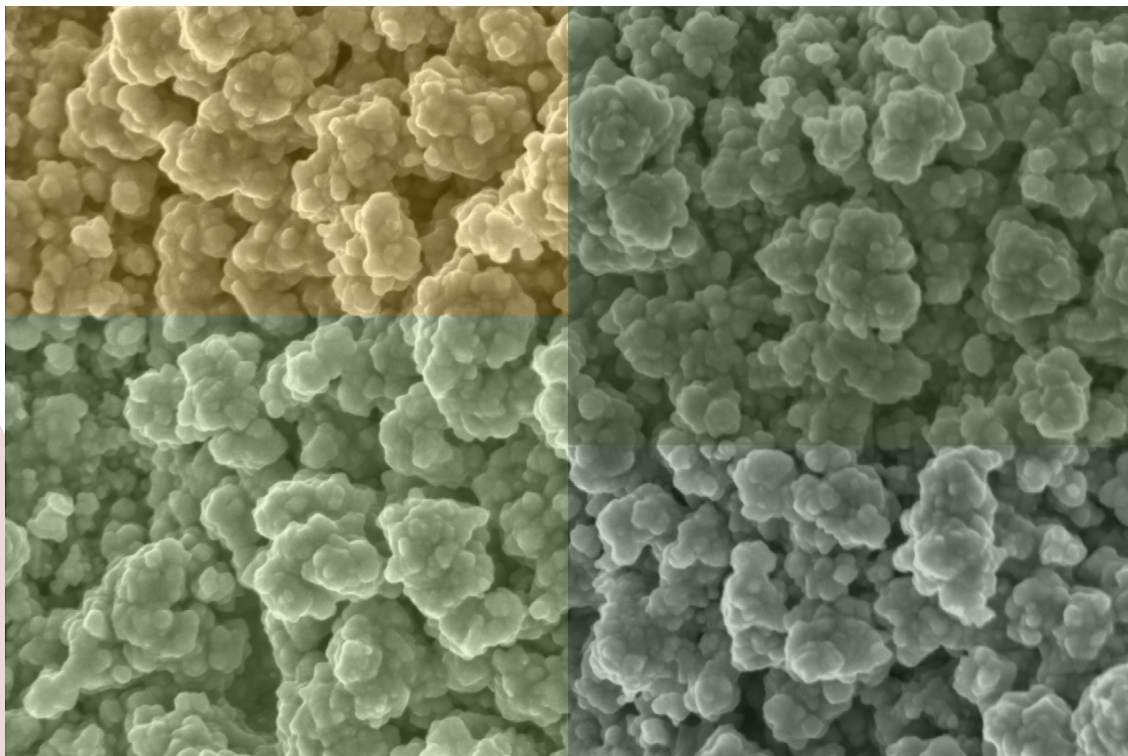


Fig. 9. (Top) Schematic representation of PEC processes on  $\text{WO}_3$  photoanode. (Bottom) (a) Variation of Faradaic efficiency of PEC generation of  $\text{S}_2\text{O}_8^{2-}$  and (b) active chlorine species on  $\text{WO}_3$  coatings during photoelectrolysis in solutions of 0.5 M  $\text{H}_2\text{SO}_4$  and 0.5 M  $\text{NaCl}$ , respectively.





# 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 the deposition of metal coatings by a controlled chemical reduction and formation of small (nano-scale) metal particles. 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 on conductors with a complicated configuration without external current. The selection of suitable reducing agents and conditions of the reaction (temperature, concentration of the reacting substances, etc.) plays a very important role in creating 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 oxidizes 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 oxidize 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 oxidized 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 employing electrochemical quartz crystal microgravimetry. The electroless metal plating method is also successively used for the 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 practical fuel cells.

## Development of catalysts for water splitting

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Electrochemical water splitting is a simple method to produce high-purity hydrogen ( $H_2$ ) through a cathodic reaction (hydrogen evolution reaction, HER) and oxygen ( $O_2$ ) through an anodic reaction (oxygen evolution reaction, OER). The electroless metal deposition has been used for the plating of the 3D binary or ternary cobalt coatings on a copper surface. The surface morphology of Co-Ni, Co-Fe, Co-Fe-Mn, Co-Fe-Mo, and Co-Zn coatings is compact and crack-free with typical globular morphology. The electroactivity of the prepared coatings towards HER and OER has been investigated in alkaline media. The lowest overpotential for the HER to reach a current density of  $10 \text{ mA cm}^{-2}$  has been found to be 128.0 mV for the Co-Fe-Mo coating. Furthermore, the lowest overpotential of 455 mV for the OER to reach  $10 \text{ mA cm}^{-2}$  also provides the Co-Fe-Mo coating. Moreover, adding Mo to the Co-Fe coating results in higher activity of the Co-Fe-Mo coating compared to pure Co-Fe. The current density increases 1.4–2.0 times increasing temperature from 25 °C to 55 °C using the prepared 3D binary or ternary cobalt coatings for HER and OER. The highest mass electro-catalytic activity of  $1.55 \text{ mA } \mu\text{g}^{-1}$  for HER and  $2.72 \text{ mA } \mu\text{g}^{-1}$  for OER has been achieved on the Co-Fe coating with a metal loading of  $28.11 \text{ } \mu\text{g cm}^{-2}$  at 25 °C.

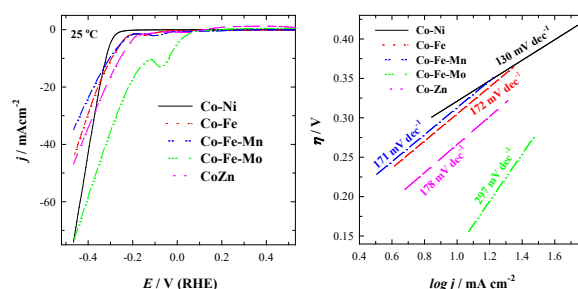


Fig. 1. (a) HER polarization curves of five studied coatings at  $5 \text{ mV s}^{-1}$  with (b) the corresponding Tafel plots. All measurements for 1 M KOH.

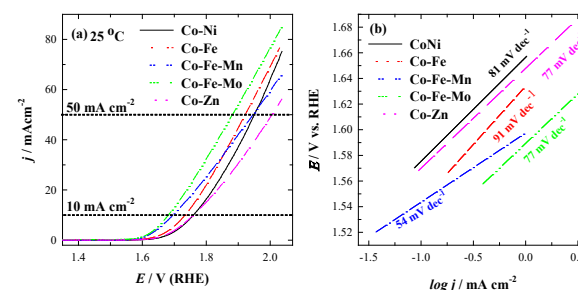


Fig. 2. (a) OER polarization curves of five studied coatings at  $5 \text{ mV s}^{-1}$  with (b) the corresponding Tafel plots. All measurements for 1 M KOH.

## Biomass-derived carbon catalysts for oxygen reduction reaction

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The use of renewable sources for energy generation is still not sufficient to meet the ever-increasing demand. Research and development of technologies for fuel cells, supercapacitors, Li- and Na-batteries, as well as improvement of their characteristics, are in a focus of attention all over the world. The carbonization of biomass residues has excellent potential to become an environmentally friendly process for the production of various products for environmental, catalytic, electronic, and agricultural applications. Hydrothermal carbonization (HTC) is an environment-friendly technology for producing a solid material named 'hydrochar'. This technology is also known as the wet pyrolysis process. The future use of these hydrochars can be tuned by intelligently controlling the product flows. In this study, an efficient non-precious electrocatalyst for oxygen reduction reaction (ORR) has been developed by hydrothermal carbonization of birch wood chips in the water under elevated pressure with subsequent activation and doping with nitrogen. The morphology of typical wavy and wrinkled layered graphene can be seen in Fig. 3. The activity of the material has been evaluated for ORR using the cyclic voltammetry (Fig. 4a) and rotating disk electrode (Fig. 4b-d) methods in 0.1 M KOH solution. The nitrogen-doped carbon material (N-HTC) was found to have a high specific surface area ( $2431 \text{ m}^2 \text{ g}^{-1}$ ) and an excellent electro-catalytic activity towards the ORR with the onset potential of 0.92 V vs RHE, showing the  $4e^-$  electrons transfer path in an alkaline 0.1 M KOH solution. Moreover, the N-HTC catalyst shows a good durability during a 1000-cycle test.

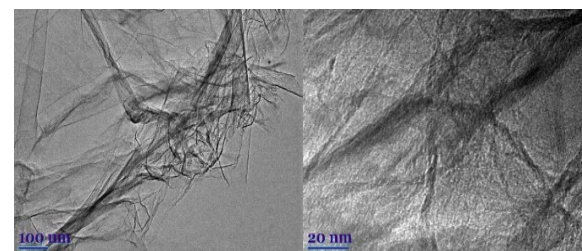


Fig. 3. TEM images of wood-derived N-doped carbon for different magnifications.

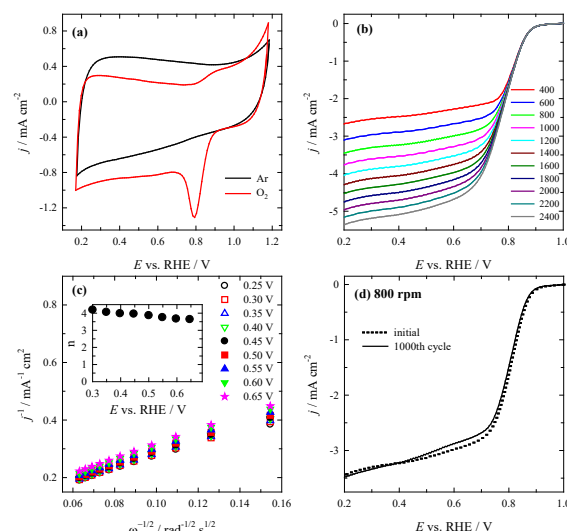


Fig. 4. (a) CVs of N-HTC in Ar-deaerated and  $O_2$ -saturated 0.1 M KOH solutions. (b) LSVs of N-HTC recorded at a scan rate of  $10 \text{ mV s}^{-1}$  in  $O_2$ -saturated 0.1 M KOH at different rotation speeds. (c) Koutecky-Levich plots at electrode potentials of 0.25–0.65 V. (d) Durability test for N-HTC at 800 rpm at  $10 \text{ mV s}^{-1}$ .



# Environment



## Investigation of the formation and life cycle of atmospheric aerosol, and its impact on climate, air quality and health

The Department of Environmental research addresses studies of the fundamental aerosol science: nucleation and growth, aerosol-light interactions, chemical and physical transformations in aerosols, multiscale modelling of aerosol properties and behaviour. Another area of Department's research is focused on source apportionment of size-resolved atmospheric aerosol particles based on number and size distribution, chemical composition and optical properties. Understanding chemical and physical processes leading to the formation of atmospheric aerosol particles is crucial to improve our capabilities in predicting the future climate and planning adaptation with mitigation strategies. Microplastics is one of the new research topics of our Department. The studies in this area aim to determine the amount of microplastic particles in different environments and characterize their morphological structure and chemical composition. Innovative methods, such as different types of degradation techniques and the application of nano-biomaterials, are also being explored in our Department to control and reduce micropollutants. A great attention is paid to the study of micropollutants (including microplastics) to determine their impact on human health. Furthermore, our scientists work on innovative and interdisciplinary research projects. By conducting the fundamental and applied research, we are aiming to find long-term solutions, especially in experimental techniques devoted to develop and apply methods determining the dynamics, balance and sources of atmospheric compounds in environmental components. Our objective is 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, understanding of key factors influencing the climate change and air quality. Department is also engaged in international and national policy-making activity.

## Evaluation of the anthropogenic black carbon emissions and deposition on Norway spruce and silver birch foliage in the Baltic region

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This study investigates potential influence of urban trees on black carbon (BC) removal by Norway spruce and silver birch along with the BC formation, mass concentration in air, and source apportionment. BC aerosol particles produced by the condensation mechanism during the combustion processes were found in all samples taken from the leaf surface (Fig. 1, Table 1). The short-term effect of BC exposure on photo-synthetic pigments (chlorophyll a and b; and carotenoids) in the foliage of one-year-old Norway spruce and silver birch seedlings was evaluated by the experiment carried out in the phytotron greenhouse. The exposure of BC particles on the spruce and birch seedlings in the phytotron increased the content of photosynthetic pigments compared to the control seedlings in the phytotron (Fig. 2). Overall, urban trees can help to improve air quality by reducing BC levels through dry deposition on tree foliage, and needle-like trees are more efficient than broad-leaved trees in capturing BC.

## Indoor-outdoor relationship of submicron particulate matter in mechanically ventilated building: Chemical composition, sources and infiltration factor

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The submicron particulate matter (PM<sub>1</sub>) generated by biomass burning (BB) and fossil fuel (FF) combustion can efficiently penetrate into the indoor environment, thus negatively affecting indoor air quality. The source apportionment results showed a dominant contribution of BB to the total carbonaceous aerosol particles, including primary (30 %) and secondary (40 %) fractions in a low-energy building with a high-efficiency filtration system. According to the enrichment factors, the main source of trace elements (TE) was road dust resuspension (30 %), while anthropogenic emissions accounted for only 13% of the trace elements. The concentrations of PM<sub>1</sub> components were significantly lower (~90%) in indoor space than in the outdoor environment (Fig. 3). The infiltration factor ( $F_{inf}$ ) of all studied PM<sub>1</sub> constituents was low ( $F_{inf} \sim 0.03$ ).

## Seasonal variation and complex analysis of microplastic distribution in different WWTP treatment stages in Lithuania

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Microplastics (MPs) pollution has become one of the most threatening environmental concerns today. Industrial wastewater, domestic wastewater, and stormwater are the three entry points for microplastics in wastewater treatment plants. Extreme weather conditions, such as rising temperatures and heavy rainfall caused by climate change, can alter the rate at which MP enters wastewater treatment plant (WWTP). In this study, wastewater and sludge samples from different treatment stages were collected during a 12-month sampling campaign (seasonal) to determine the efficiency of a municipal wastewater treatment plant in removing MP particles (Fig. 4). MPs in a range of 20 - 1000 µm were detected and classified by shape, color, size, and chemical composition depending on the season and treatment stage (Fig. 5). The average removal rate in the WWTP was 57 %

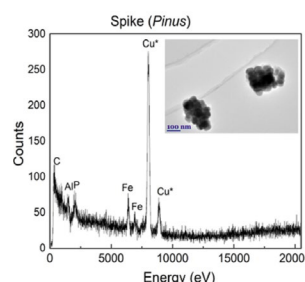


Fig. 1. TEM images and EDX spectra of black carbon containing particles found on leaves and needles.

Table 1. Diameter of primary particle, length and width of black carbon agglomerate.  $\phi$  - diameter of primary particle, L and W is the maximum length and width of agglomerate.

|          | $\phi$ , nm | L, nm | W, nm |
|----------|-------------|-------|-------|
| Leaf-1   | 24          | 234   | 132   |
| Leaf-2   | 23          | 130   | 80    |
| Leaf-3   | 30          | 97    | 69    |
| Needle-1 | 32          | 176   | 177   |
| Needle-2 | 41          | 273   | 20    |

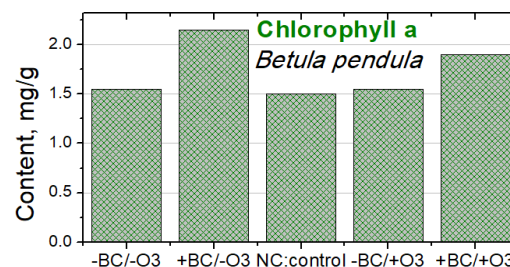


Fig. 2. Chlorophyll a (mg/g) in the foliage of silver birch (*Betula pendula*) seedlings under different growing conditions.

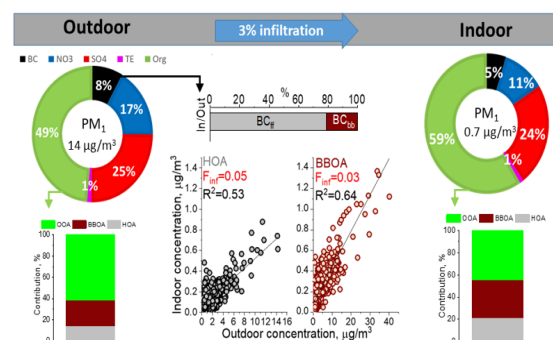


Fig. 3. A schematic diagram of the investigated indoor/outdoor parameters. Here  $F_{inf}$  is the infiltration factor, TE- trace elements, BBOA- biomass burning OA, HOA- hydrocarbon-like OA, OOA-oxygenated OA.

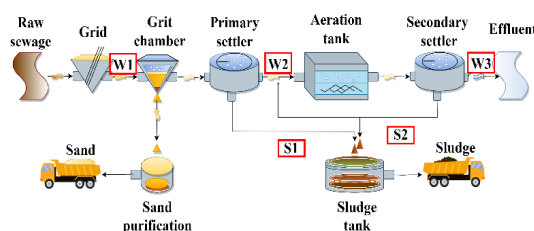


Fig. 4. Schematic diagram of the main stages of the WWTP and the sampling points (W1 – influent wastewater, W2 – first treatment stage, W3 – second treatment stage (effluent), S – sewage sludge).

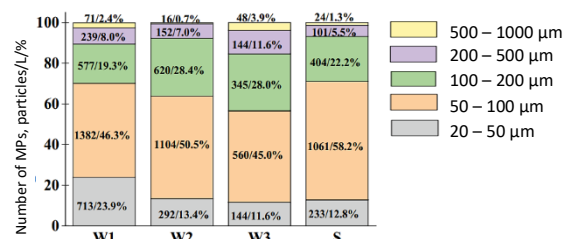
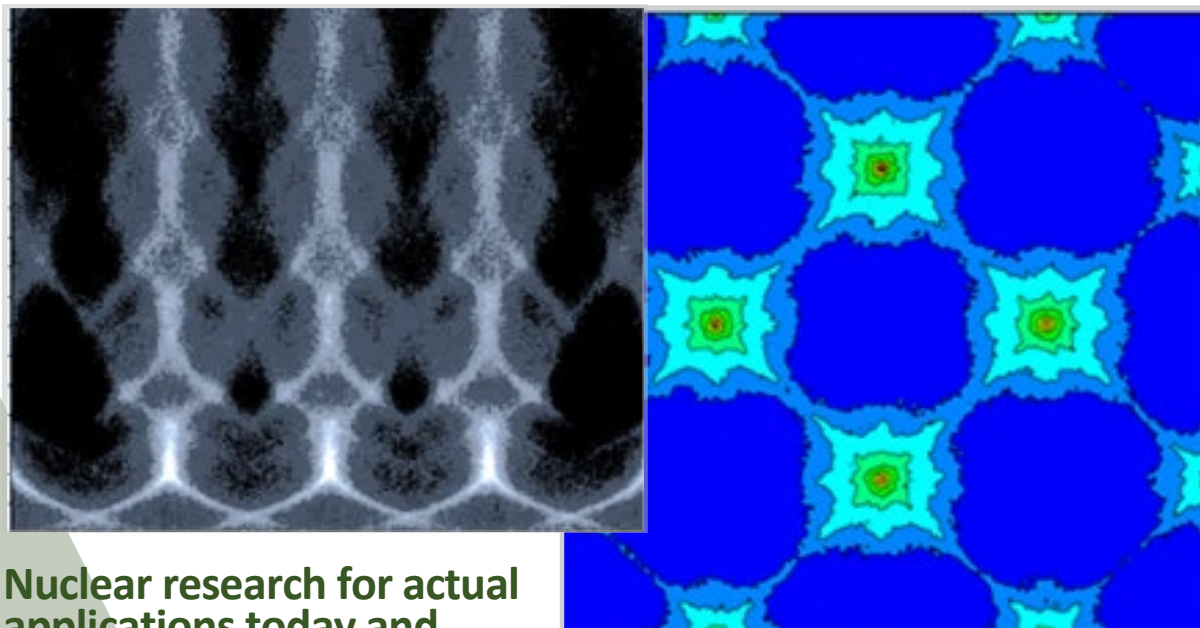


Fig. 5. Abundance and size distribution of microplastics in different WWTP treatment stages during the spring season.



# Nuclear



## Nuclear research for actual applications today and innovative technologies for future

The Department of Nuclear Research is involved in development and application of known and innovative methods in the fields of nuclear fuel cycle technologies, experimental nuclear and mass spectroscopy, ion beam application for material analysis and applications of lasers for generation of ionizing radiation. Optimization of nuclear facility radioactive waste management (RWM) and comprehension of processes of radionuclides transport through engineering barriers to enable nuclear facility safety are key applications of nuclear research carried out in the *Experimental Nuclear Research Laboratory*. Participation in multinational RWM projects allows to gain and to use modern practice of RWM technology, knowledge of RW predisposal and deep geological disposal management. Development of ion beam methods for material analysis and modification is important part of our activities having intersection both with semiconductor materials and applications for lasers. Investigation of organic scintillator films opens new possibilities of inexpensive material application for detection and spectroscopy of ionizing radiation particles. The principles of high energy electromagnetic radiation generation are investigated using ultrashort laser pulses, taking into account practical application possibilities. Complementary information on material properties (magnetic properties, oxidation and corrosion of iron compounds) is determined by Mössbauer spectroscopy. In the *Isotopic Research Laboratory* our attention is focused on environmental impact assessment of energy generating facilities, effects of land-use change and urban development on carbon sequestration in different environment. Aspects of isotopic niches of small organisms, source apportionment of carbonaceous aerosol from forested sites and a multi-isotope approach for contaminant monitoring are also investigated. Application of a stable isotope ratio analysis ( $\delta^{13}\text{C}$ ,  $\delta^{15}\text{N}$ ,  $\delta^{18}\text{O}$  and  $\delta^{34}\text{S}$ ) in environmental, archeological and food samples is implemented and it stimulates new promising technologies.  $^{14}\text{C}$  measurements are performed in *Accelerator Mass Spectrometry Laboratory*. These studies open potentially new field of activity related to carbon dating and analysis of triple carbon ratio for dedicated samples. Close collaboration of our laboratories stimulates the development of smart-environmental and environment-safe nuclear fuel cycle technologies and implementation of new material modification and analysis methods for public and business needs.

## Optimization of radioactive waste (RW) management technologies

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In the blind benchmark exercise, the values of decay heat rate of five spent nuclear fuel assemblies, obtained by various participants based on the same irradiation description and validated with measured value, were compared (Fig. 1). This experiment has led to performing a first assessment of up to date simulation capabilities, as well as current prediction potentials. Very low level radioactive waste (VLLW, i.e. above clearance level) does not require high level of containment and isolation being suitable for disposal in near surface landfill type facilities with limited regulatory control. After careful inspection procedure, it could possibly meet exempt waste criteria for clearance (effective per year doses to individuals should be of the order of 10  $\mu$ Sv or less). For this waste characterization, the methods like in-situ nuclear spectroscopy and dose rate measurements, such as waste inventory by NV determination procedure, are needed. A very low level of radioactive waste, radioactive near surface landfill, has been found at Ignalina nuclear power plant site by experimental survey using  $\text{CeBr}_3$  gamma spectrometer, MCNP6 modeling tool for detector efficiency estimation and NV confirmation for clearance possibility evaluation (Fig. 2a). Assessment of dose rate of activated PWR vessel and radiation protection shielding containers was performed using MCNP modeling for final management project of Paldisky low and intermediates level radioactive waste site (Fig. 2b).

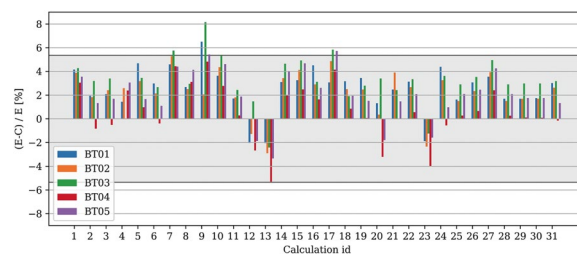


Fig. 1. Relative difference between measured (E) and calculated (C) decay heat rate values for five different PWR assemblies.

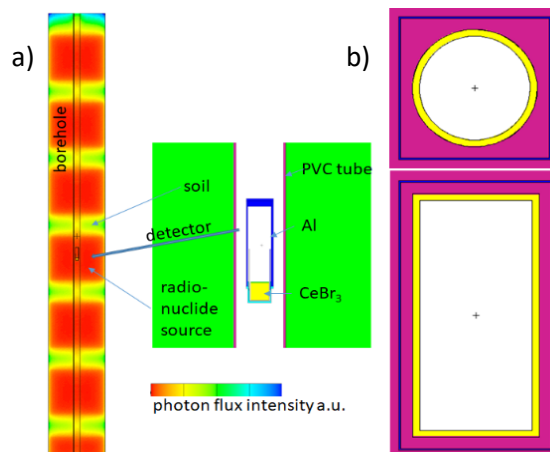


Fig. 2. (a) Modeling of  $\text{CeBr}_3$  detector response in the radioactive waste surface landfill repository borehole. (b) Model cross-sections of the PWR /BM-A (70MW) reactor vessel and its rectangular radiation protection concrete container (thickness 3 cm).

## Radiocarbon generation and atmospheric release assessment from nuclear power plant with RBMK type reactors

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We obtained a comprehensive understanding of  $^{14}\text{C}$  nuclide generation and release from the main circulation circuit and gaseous circuit of RBMK-1500 reactors operated at Ignalina NPP. The primary sources of  $^{14}\text{C}$  generation and airborne release are evaluated as 0.491 and 0.367 TBq per one calendar year (10.5 months of effective reactor operation at 1350  $\text{MW}_e$  power), respectively. The analysis of the operation specifics of these systems demonstrated that they do not provide an effective barrier to contain  $^{14}\text{C}$  due to the  $^{14}\text{CO}_2$  chemical form of radiocarbon in RBMK reactors, i.e., 100% release (0.858 TBq/year) have been evaluated available for atmospheric release. These results have been compared to the atmospheric releases evaluated from the  $^{14}\text{C}$  activity concentration measured in pine tree ring samples by single stage accelerator mass spectrometer (SSAMS, NEC, USA) at AMS laboratory, resulting to airborne release value of 1 TBq/year for one RBMK-1500 reactor. Slightly higher value reproduced from the tree ring samples indicates that the reactor graphite stack might be also a source of the  $^{14}\text{C}$  releases of about  $0.14 \div 0.24$  TBq/year. Based on similar design features, the results of our study can be easily projected on the RBMK-1000 reactors rescaling  $^{14}\text{C}$  source term according to the lower reactor power.

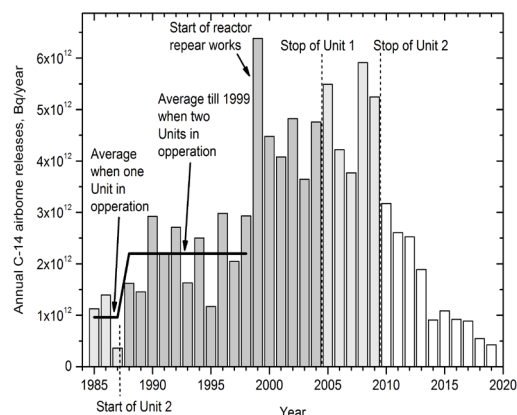


Fig. 3. (Top) Ignalina NPP site. (Bottom) Annual  $^{14}\text{C}$  releases from Ignalina NPP to air based on the  $^{14}\text{C}$  concentration measurements in pine tree rings.



## Investigation of anthropogenic radionuclides at aqueous and soil environment

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Radiocesium and plutonium isotopes are commonly found in the environment as a result of nuclear weapons tests or accidents at nuclear facilities. Accurate and reliable determination of the concentration of  $^{137}\text{Cs}$  and Pu isotopes in the environmental samples is important due to the potential hazard of these radionuclides to human health. New method of concentration measurement of radionuclides from aqueous environment using raw and modified biosorbents (moss *Ptilium crista - castrensis* and oak sawdust *Quercus robur*, both in the form of natural and modified state) was developed, the main functional groups and sorption mechanisms have been identified. It was shown, that the biosorbent modification significantly increases the sorbent surface area (see Fig. 4). The best results for the sorption were shown by carbonated sawdust activated with HCl for Cs and raw moss and moss modified with iron hydroxide for plutonium. The migration capabilities of  $^{137}\text{Cs}$  and  $^{239,240}\text{Pu}$  in the soil layers have been studied by sequential extraction determining the geochemical forms of radionuclides of non-boggy and waterlogged soil cores sampled on the shores of lake Bedugnys. The value of the exchangeable fraction of radionuclides is shown to be indicative of their migration capabilities in vertical profile of the soil.

## Effect of lanthanide (La, Ce, Pr, Nd) substitution on structural and magnetic properties of $\text{Y}_3\text{Fe}_5\text{O}_{12}$

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Ferrimagnetic yttrium and rare-earth iron garnets demonstrate high resistivity which makes them suitable for high frequency applications. The garnet structure has three different lattice sites for cations, therefore, the properties of  $\text{Y}_3\text{Fe}_5\text{O}_{12}$  can be modified by substitution of cations either in tetrahedral and octahedral sites occupied by iron or dodecahedral sites occupied by yttrium. In this study, the substitution of yttrium by four lanthanides (La, Ce, Pr and Nd) yttrium was performed in the samples synthesized by the sol-gel method. The XRD and Mössbauer spectroscopy data (Fig. 5) demonstrate that the substitution with lanthanides affects the phase composition of obtained samples. High substitution levels lead to the formation of large amount of antiferromagnetic perovskite and hematite phases. However, for intermediate levels

## Automated method for thermal-optical separation of aerosol organic/elemental carbon for $^{13}\text{C}$ analysis

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A method for  $^{13}\text{C}$  analysis in different fractions of carbonaceous aerosols, especially elemental carbon (EC) was evaluated. This method combines a Sunset thermal-optical analyzer and an isotope ratio mass spectrometer (IRMS) via a custom-built automated separation, purification, and injection system. Organic carbon (OC), EC, and other specific fractions from aerosol filter samples can be separated and analyzed automatically for  $^{13}\text{C}$  based on thermal-optical protocols (EUSAAR\_2) at sub- $\mu\text{gC}$  levels. The main challenges in isolating EC for  $^{13}\text{C}$  analysis are the possible artifacts during OC/EC separation, including the premature loss of EC and the formation of pyrolyzed OC (pOC) that is difficult to separate

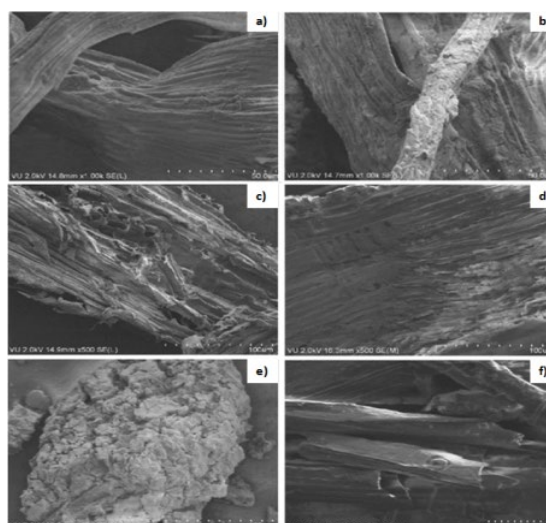


Fig. 4. SEM images of (a) raw moss, (b) moss modified with iron hydroxide, magnification  $\times 1000$ , (c) raw sawdust, (d) sawdust modified with iron hydroxide, (e) sawdust after carbonization at  $300^\circ\text{C}$  temperature and (f) carbonized sawdust modified with HCl, magnification  $\times 500$ .

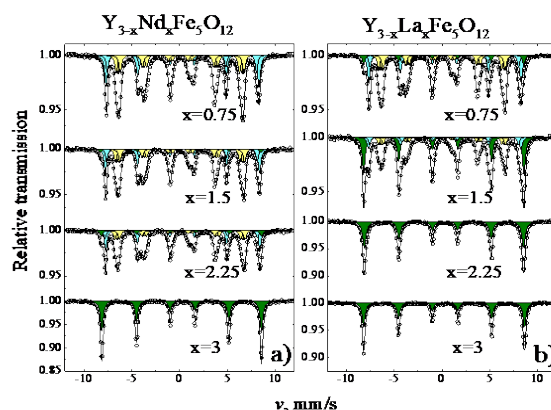


Fig. 5. Dependence of Mössbauer spectra of (a)  $\text{Y}_{3-x}\text{Nd}_x\text{Fe}_5\text{O}_{12}$  and (b)  $\text{Y}_{3-x}\text{La}_x\text{Fe}_5\text{O}_{12}$  on amount of substitution. Yellow and cyan denote garnet phase, while olive is due to perovskite and hematite phases.

of substitution with heavier lanthanides Nd and Pr, the garnet phase remains dominant. These results are also confirmed by saturation magnetization and coercivity measurements.

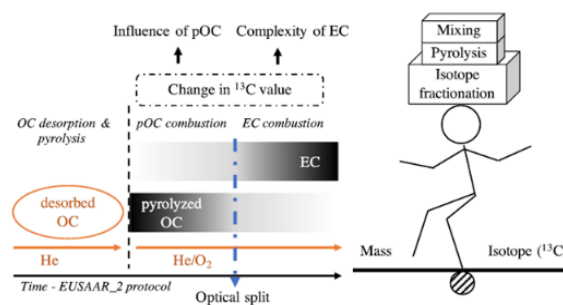


Fig. 6. A schematical representation of the automated method.

from EC. Since those artifacts can be accompanied by isotope fractionation, their influence on the stable isotopic composition of EC was comprehensively investigated with various test compounds. The results show that the thermal-optical method is relatively successful in OC/EC separation for  $^{13}\text{C}$  analysis.

## Development of graphitization method for low carbon aerosol filter samples

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The wide applications of the radiocarbon ( $^{14}\text{C}$ ) approach in environmental, archeological, and geological research often necessitates the analysis of microgram-sized samples. The ability to measure low carbon samples is particularly relevant for aerosol particle filters. Here, the dilution method is used for aerosol source apportionment studies as much faster and less filter requiring than conventional methods. The determination of  $^{14}\text{C}$  values of aerosol filters with low carbon content (starting at  $40\text{ }\mu\text{g C}$ ), previously unfeasible with the current AGE-3 system, are now possible. We used sample dilution method for graphitization of low-carbon samples ( $20\text{--}200\text{ }\mu\text{g C}$ ) with an Automated Graphitization System, AGE-3, and applied a mass balance equation for the calculation of  $^{14}\text{C}$  values. This method does not require sample weighing, as the elemental analyzer measures the area of the sample  $\text{CO}_2$  with greater accuracy. Further this is used for calculations of the  $^{14}\text{C}$ . The established confidence limits of the method are  $\pm 2\text{ pMC}$ , insignificant for estimation of partial inputs of different aerosol sources.

## Impacts of land-use change and urban development on carbon sequestration in tropical seagrass meadow sediments

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Seagrass meadows store significant carbon stocks at a global scale, but land-use change and other anthropogenic activities can alter the natural process of organic carbon ( $\text{C}_{\text{org}}$ ) accumulation (Fig. 8). The carbon accumulation history of two seagrass meadows with different degrees of disturbance in Zanzibar (Tanzania) was assessed. It was shown that seagrass meadows accumulated  $\text{C}_{\text{org}}$  at an average rate of  $22\text{--}25\text{ g C}_{\text{org}}\text{ m}^{-2}\text{ yr}^{-1}$  over the last  $\sim 80$  years, and stored substantially higher amounts of  $\text{C}_{\text{org}}$  relative to the unvegetated site. It was concluded that land-based human activities have modified the carbon storage of seagrass meadows in Zanzibar and ongoing coastal transformation might change the  $\text{C}_{\text{org}}$  storage capacity of seagrass ecosystems due to altered organic matter sources and increased accumulation rate (by  $24\text{--}30\%$ ). This highlights the necessity to consider the land–sea interface (including coastal development) and habitat connectivity to better understand the blue carbon capacity of the coastal zone. The results of this study can be used to guide coastal management for protection of seagrass meadows as sinks of atmospheric  $\text{CO}_2$ .

## Seasonal observation and source apportionment of carbonaceous aerosol

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The dependence of stable carbon isotopic ratio ( $\delta^{13}\text{C}_{\text{TC}}$ ) variation on air mass direction at the hemiboreal forest site (Lithuania) during the cold and the warm seasons demonstrated the differences of  $\delta^{13}\text{C}_{\text{TC}}$  that could be primarily attributed to different sources and seasons (Fig. 10). Source apportionment of organic aerosol (OA) measurement with ACSM using PMF analysis yielded a three-factor solution: biomass-burning related OA (17%), more oxygenated OA (52%), and less oxygenated OA (31%). Our analysis highlights the importance of comprehensive identification of possible regional aerosol particle sources.

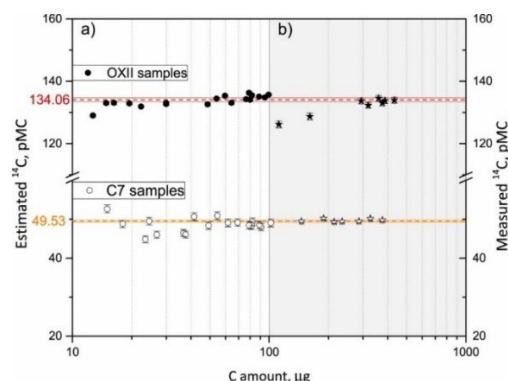


Fig. 7. Estimated and measured pMC values of samples with known pMC: (a) prepared and measured by dilution method (carbon amount  $15\text{--}100\text{ }\mu\text{g}$ ) and (b) measured  $^{14}\text{C}$  values of the samples prepared using the conventional method (carbon amount  $100\text{--}500\text{ }\mu\text{g}$ ). The red line shows the nominal pMC values for investigated samples.

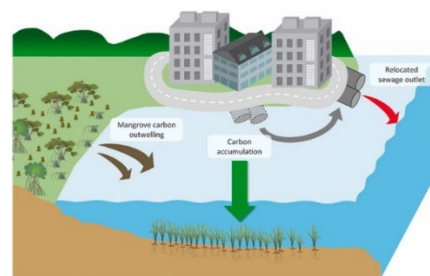


Fig. 8. Schematic diagram of investigated processes.

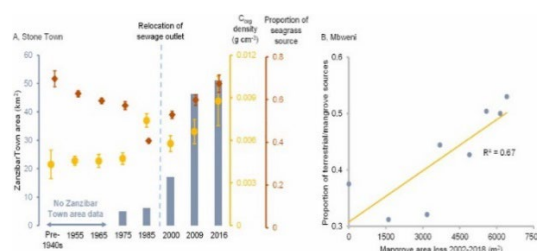


Fig. 9. (Left) Land-use areal expanse of Zanzibar Town since 1975 and the relocation of sewage outlet in the mid-1990s against the  $\sim 10$  years mean ( $\pm\text{SE}$ ) of  $\text{C}_{\text{org}}$  density and proportion of seagrass source input in Stone Town seagrass sediments for the different time periods. (Right) Loss of mangrove area during 2002–2018 in relation to the proportion of mangrove/terrestrial sources in the sediment of the Mbweni seagrass site.

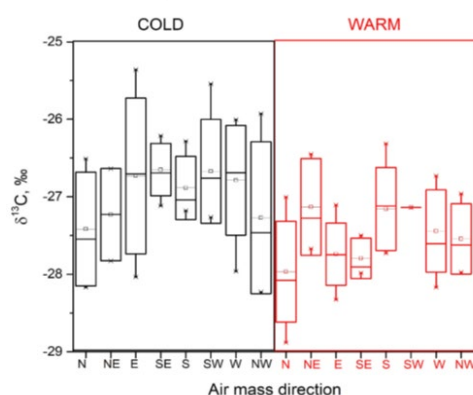
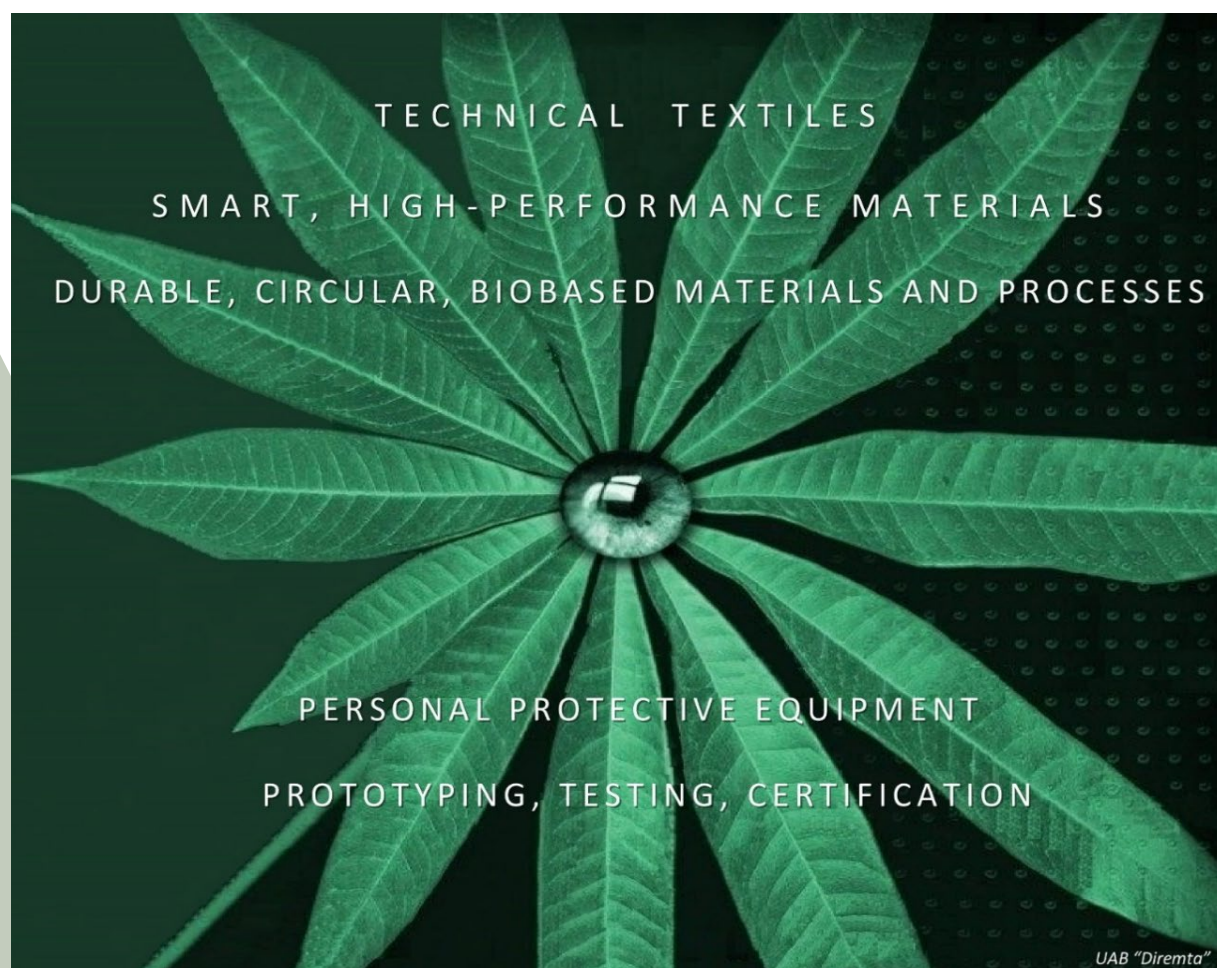


Fig. 10. Dependence of  $\delta^{13}\text{C}_{\text{TC}}$  variation on air mass direction at the hemiboreal forest site during the cold and the warm seasons.



# Textile technologies



## The Department of Textile Technologies

Interactions between textile materials, human health, and environmental impact are highly complex, dynamically changing over time and requiring comprehensive research. Department of Textile technologies following the research priorities of EU Strategy for Sustainable and Circular Textiles continued its scientific activities in developing new, low footprint products and processes. In cooperation with industry partners the biodegradable and natural fiber based materials were developed. The focus was on reducing the negative effects of textile processing: scientific research of low-pressure plasma treatment impact on biobased fabric finishing was carried out. Developing of smart and high-performance products for military application remained the core of the research in the department. System and method for personal thermal comfort of smart ballistic protection equipment with active thermoregulation system was applied and registered in European patent office. Research and development of adaptive camouflage techniques was continued, and new project proposal was submitted for EU European Defence Fund. For further development of smart, high-performance materials, digital printing technology was implemented, and laboratory digital printer and spectrophotometer were approved for financing by Research Council of Lithuania. This would enhance the range of our research from the novel idea to prototyping of innovative products.

## Impact of low-pressure plasma treatment of wool fabric for dyeing with PEDOT: PSS

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This study demonstrates the effect of non-thermal plasma modification to surface morphology, color characteristics and electrical conductivity of wool fabric dyed with intrinsically conductive polymer (ICP) poly (3, 4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT: PSS). The wool fabric was treated with an aqueous dispersion of PEDOT: PSS, Clevios F ET, providing electrically conductive properties to textiles. The wool fabric, containing basic groups of amine ( $-\text{NH}_2$ ), was pre-activated at 90 °C with low-pressure plasma of non-polymer forming nitrogen ( $\text{N}_2$ ) gas before exhaust dyeing with PEDOT: PSS. This treatment enhanced hydrophilicity, reduced felting, increased adhesion, improved dye ability and ensured more PEDOT: PSS negatively charged sulfonate ( $-\text{SO}_3^-$ ) counter ions to be electrostatically bounded with the cationic protonated amine groups of the wool fiber. Initially, before  $\text{N}_2$  gas plasma treatment and after fabrics were evaluated according to the test method for aqueous liquid repellency, the surface morphology of the plasma-modified and unmodified wool dyed fabric was observed with scanning electron microscopy (SEM) (Fig. 1). The functional groups, introduced onto the surface after  $\text{N}_2$  gas plasma treatment of wool fabric, were characterized by X-ray photoelectron and FTIR-ATR spectroscopy

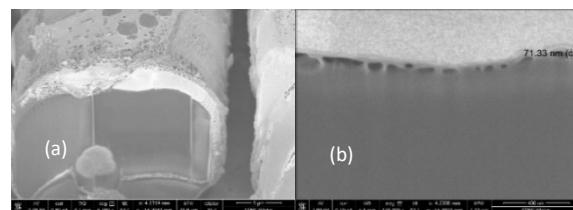


Fig. 1. SEM images of  $\text{N}_2$  plasma-modified and dispersed in aqueous solution of PEDOT: PSS, Clevios F ET, dyed wool fiber. Cross section: magnification (a) x6500 and (b) x120000.

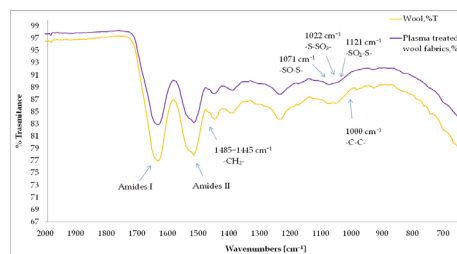


Fig. 2. FTIR-ATR spectra illustrating untreated and  $\text{N}_2$  gas plasma-treated wool fabrics.

(Fig. 2). The results of color difference measurements show that  $\text{N}_2$  gas plasma treatments provide more intense color on Clevios F ET dyed wool fabric and retain its electrical conductivity.

## Prediction of air permeability coefficient and water-vapor resistance of 3D textile layer

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A computational model for investigation of the air permeability coefficient and the water-vapor resistance coefficient of 3D textile layer (Fig. 3) is presented. The effective values of the coefficients are highly dependent on the volumetric internal structure of the layer. The computational study of air and water vapor flow has been performed using the micro scale finite element model of the representative volume of the textile layer by considering the real configuration of the yarns and filaments. The unit cell models (Fig. 4) of specific textile layers were developed to simulate the physical processes influencing the air permeability and water-vapor resistance coefficients of the fabrics. The Model 6 was used for the representation of two-layer woven fabric combined of two replicas of the Model 3. The dimensions of air domain in Models 1, 3, 5, 6, 7 were 1.4 mm x 1 mm x 10 mm and the thickness of textile layer domain was 0.439 mm. The dimensions of the air domain in Models 2 and 4 were 1.05 mm x 1 mm x 10 mm and the thickness of the textile layer domain was 0.438 mm. Model 7 was equivalent to the 3D textile layer and represented unit cell model, where top and bottom layers are based on Model 6 and combined together with spacer yarn. In Models 5, 6, 7 the distance between two textile layers was 3.06 mm. In Model 7 the radius of spacer yarn was 0.08 mm. The spacer yarn is made from polypropylene with linear density 18 tex. The effective values of the coefficients were obtained by taking average values of air and water vapor fluxes through the thickness of the representative volume. The steady state computational models in micro scale are based on Navier-Stokes and Brinkman partial differential equations. The simulations were performed in Comsol Multiphysics software environment by using laminar flow application mode. Numerical results for the air permeability of the samples were obtained, analyzed and validated comparing with the experimental data, and good agreement has been achieved (Fig. 5).

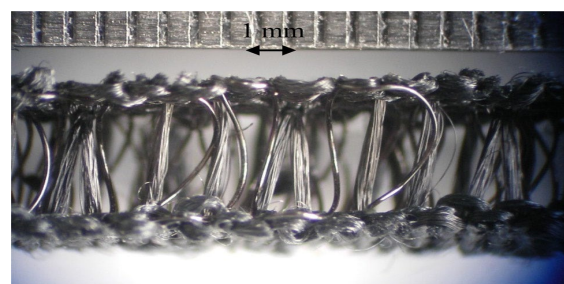


Fig. 3. The sample of 3D textile.

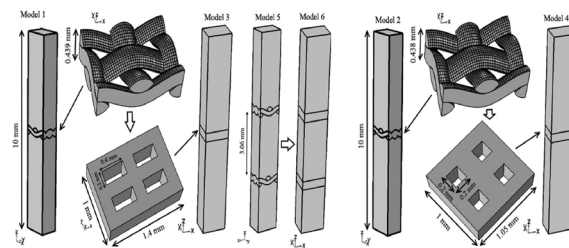


Fig. 4. Geometry of Models 1–6.

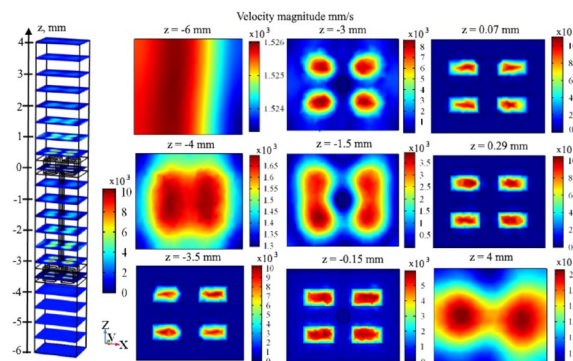
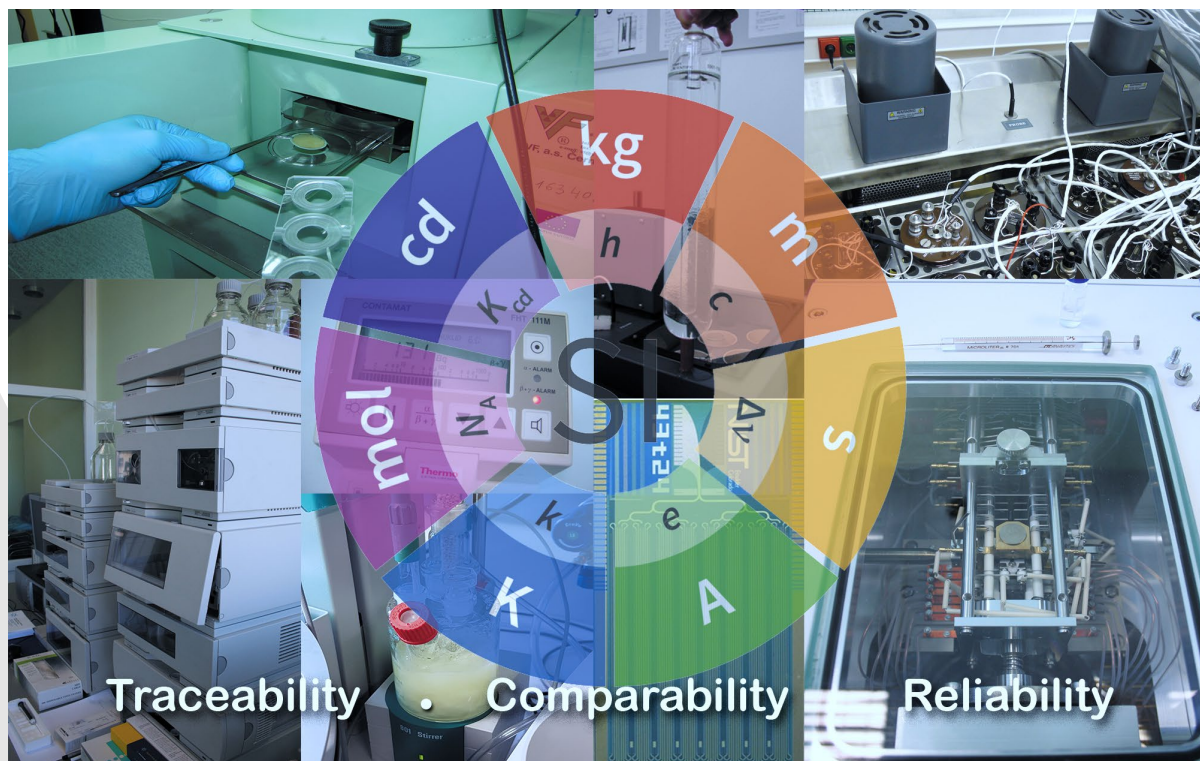


Fig. 5. Simulation results of Model 7: Distribution of the velocity flow.



# Metrology



## National Metrology Institute of Lithuania

Metrology is the science of measurement and its application. In metrology one has to deal with correctness, accuracy and reliability of measurement results. The core of metrology lies in the validation of the result, particularly by specifying its actual limitations.

FTMC was authorized to perform and implement functions of the National Metrology Institute (NMI) since 1 July 2014. The Quality Management System (QMS) was created fulfilling the requirements of the international standard ISO/IEC 17025:2017. The QMS was peer-reviewed on a periodical basis which was recognised by EURAMET. In 2021, the NMI of Lithuania became one of eight NMIs of Nordic-Baltic countries which established European Metrology Network (EMN) *Smart Specialisation in Northern Europe*.

Currently, FTMC maintains the national standards in the following areas of measurements: electricity and magnetism, ionising radiation, length, mass, metrology in chemistry, thermometry, time and frequency.

**Time and Frequency Standard Laboratory (TFSL)** is reproducing values of the unit of time, the second (s), and the unit of frequency, the hertz (Hz). The mission of TFSL is the 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 qualified time stamping services which meet the eIDAS regulations and the ETSI standards. The time stamping service issued up to two million time stamps per month for Lithuanian governmental organisations and European users.

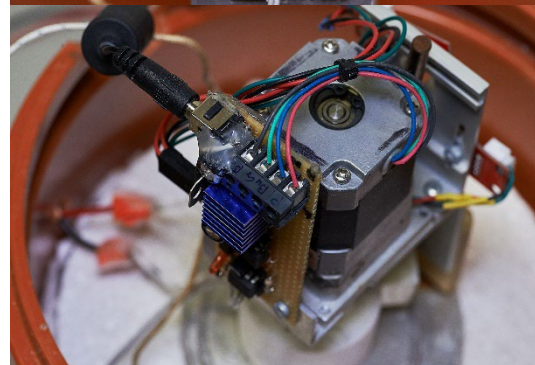
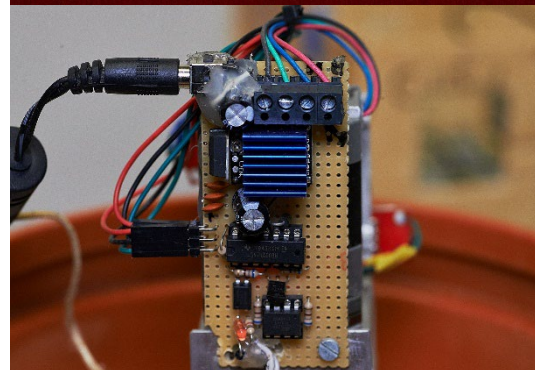
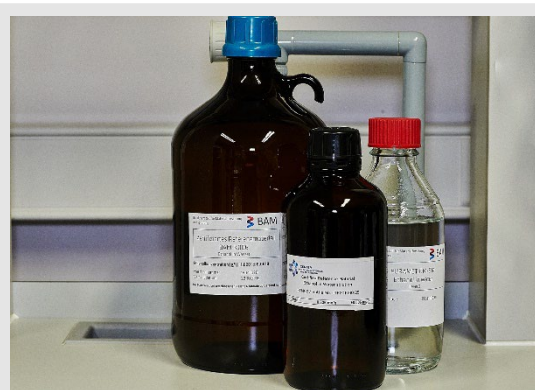
The mission of the **Electrical Standards Laboratory (ESL)** is maintaining and developing the standards of unit of voltage, the volt (V), and unit of resistance, the ohm ( $\Omega$ ), ensuring their traceability to the SI, calibrating working standards and measurement devices, pursuing research in the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

The mission of the **Temperature Unit Standard Laboratory (TUSL)** is the realization of the international temperature scale ITS-90 and the value of the unit of temperature, the Kelvin (K), ensuring their traceability to the SI. Lithuanian National Standard of the temperature unit (in the range from  $-195^{\circ}\text{C}$  to  $+961,78^{\circ}\text{C}$ ) is of the primary level while the reference point of the freezing point of Cu ( $+1084,62^{\circ}\text{C}$ ) is of the secondary level.

Both the national standard of mass and the national standard of length were transferred to FTMC by the Government of the Republic of Lithuania in 2019. The mission of the national gauge blocks standard is maintaining and transferring length unit (in the range from 0,5 mm to 100 mm) ensuring its metrological traceability to the SI system. The mission of the national mass unit standard is maintaining and developing the standards of mass unit ensuring the traceability to the SI system in the range from 1 mg to 20 kg. The reference equipment can also measure the magnetic properties and density of weights.

The reliable, traceable and accurate chemical measurements in different sectors of biotechnology, healthcare, safety and environment protection is provided by the **Laboratory for Metrology in Chemistry (LMiC)**. In 2022, the LMiC continued its activities in a new research project *01.2.1-LVPA-K-856-01-0120 "Development of in-combo methods for the evaluation of the safety of compounds for humans and environment and development of products prototypes based on them"*. The project develops prototypes for new products characterizing chemical compounds applied in chemistry, cosmetics and pharmaceutical industry. Another area of laboratory interests is a new regional metrological capacity for certification of reference materials according to the requirements of ISO 17034 standard, as well as research in the field of volatile organic compounds for different applications.

The **Ionizing Radiation Metrology Laboratory (IRML)** participated in the IAEA-TERC-2022-01/02 *World-wide open Proficiency Test on determination of anthropogenic and natural radionuclides in water, soil (gamma-ray spectrum analysis exercise), and simulated contaminated surface samples* organized by the International Atomic Energy Agency (IAEA). The TRIC 2022 Test on tritium activity measurement in water was also organized by the IAEA. The IRML continued planned activities within the EMPIR 2020 joint project 20SIP02 on dissemination of the pre-selection and free release measurement technology to the end-users from nuclear facilities. The calibrations and sample measurements, ensuring traceability to the National Standard of radionuclide activity, were carried out for Lithuanian hospitals and other customers.





# Open access facilities

## Electron microscopy, X-ray spectroscopy and XRD open-access center (OAC)

→ <https://litexbeam.ftmc.lt>

OAC offers open access facilities for characterisation of solid material surface structure, morphology, inner and crystalline structure, chemical and phase composition. The OAC infrastructure has been improved significantly during last 10 years, and now is equipped with modern electron microscopes (FE-SEM-FIB and TEM), X-ray diffractometers, X-ray fluorescence (WD-XRF), X-ray photoelectron (XPS) and Auger electron spectrometers. The OAC provides characterisation services of solid materials for customers from academic institutions and industry in Lithuania and abroad. Among the customers, there are universities of Southampton, Hoseo (South Korea), Riga, Vilnius and Kaunas. OAC provided structure characterisation services for such companies as Translucent Inc (from Palo Alto), IQE (North Carolina), Brolis Semiconductor, Altechna, Optolita and many others.

## Prototype formation and integration

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### 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) micro-processing line has started to function. It is ready to produce the working models and the demonstration proto-types 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 MoS<sub>2</sub>, multi-mode magnetron sputtering for deposition of multicomponent functional films and molecule beam epitaxy for GaAs based optoelectronic devices.

**The CR services include:** 1) CR (ISO7–ISO5 about 300 m<sup>2</sup>) 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 OAC 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 nanometre scale level and the level of the complete unit.

**The characterization includes:** 1) topography, force spectroscopy, tunnelling 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.



## BALTFAB processing technologies

→ <http://www.baltfab.com/>

BALTFAB is a joint open user facility between departments of Laser technologies and Nanoengineering, 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 microfabrication workstations are equipped with full variety of industrial ns-, ps- and fs- lasers. The BALTFAB team include 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.

**Services include:** 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:** Multi-axis workstations with ultra-short pulse lasers for experimentation, rent and user training services. Dip pen nanolithography and imaging ellipsometry for creating and imaging of molecular surfaces.

## Converse and chemical coatings

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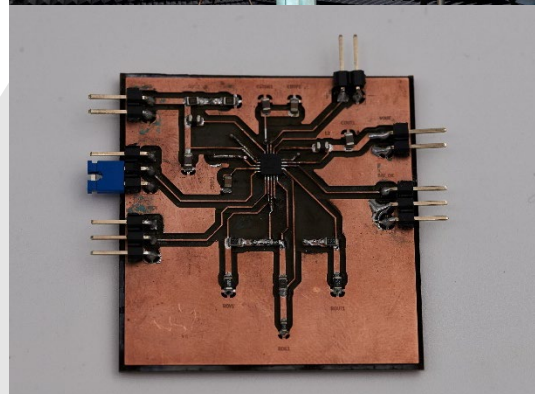
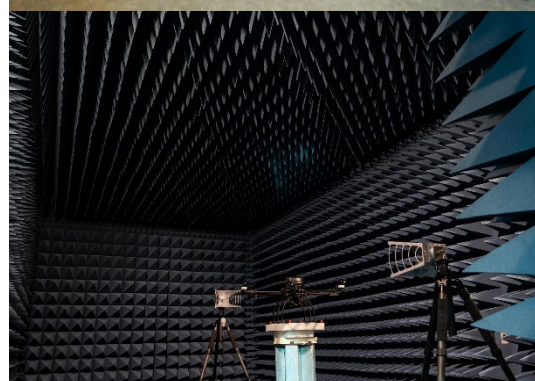
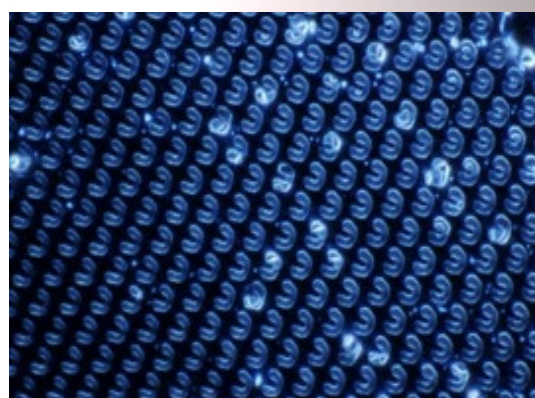
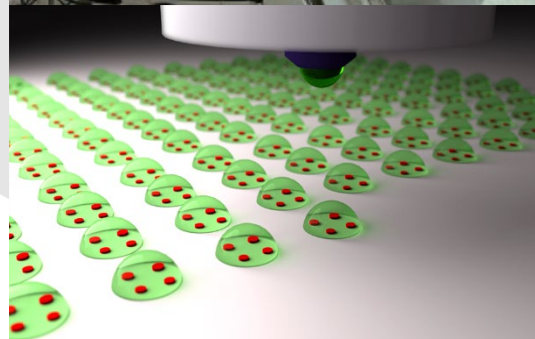
specializes in aluminium and its alloys anodization, galvanic precious metals plating and related fields. The services provide: electrodeposition of protective, decorative as well as technical converse (anodic) coatings, structural etching of decoration elements, adsorption colouring of anodized surfaces, modify-cation of aluminium and its alloys surfaces with a passivation film that ensures 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.

## Microwave transmission, reflection and absorption

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In the new microwave anechoic chamber we developed a setup for microwave transmission and reflection measurement in a frequency range from 1 GHz to 18 GHz. 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.





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☐ The most frequently used keywords in publications in 2022.

**with FTMC affiliations in 2022  
in the top quartiles (Q1-Q4) journals**

- 11.** Anulytė, J.; Bužavaitė-Vertelienė, E.; Stankevičius, E.; Vilkevičius, K.; Balevičius, Z. High spectral sensitivity of strongly coupled hybrid Tamm-plasmonic resonances for biosensing application // *Sensors*. Basel: MDPI AG. eISSN 1424-8220. 2022, vol. 22, iss. 23, art. no. 9453, p. 1-10.

12. Anulytė, J.; Bužavaitė-Vertelienė, E.; Vertelis, V.; Stankevičius, E.; Vilkevičius, K.; Balevičius, Z. Influence of a gold nano-bumps surface lattice array on the propagation length of strongly coupled Tamm and surface plasmon polaritons // *Journal of materials chemistry C*. Cambridge: Royal Society of Chemistry (RSC). ISSN 2050-7526. 2022, vol. 10, iss. 36, p. 13234-13241.
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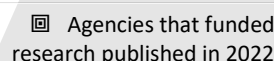
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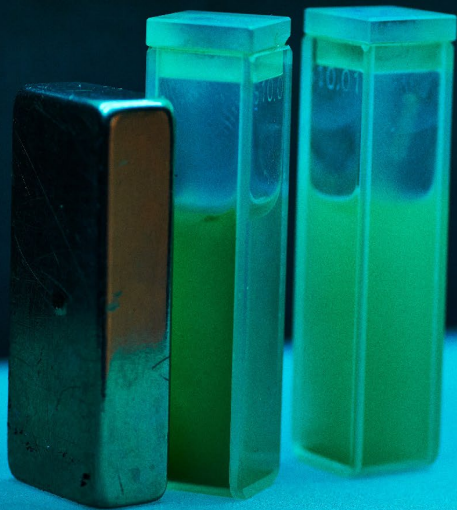
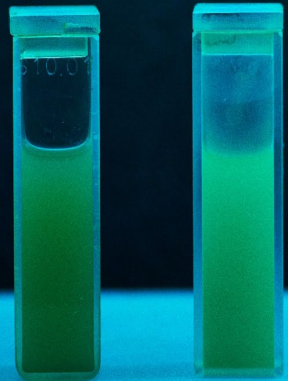
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