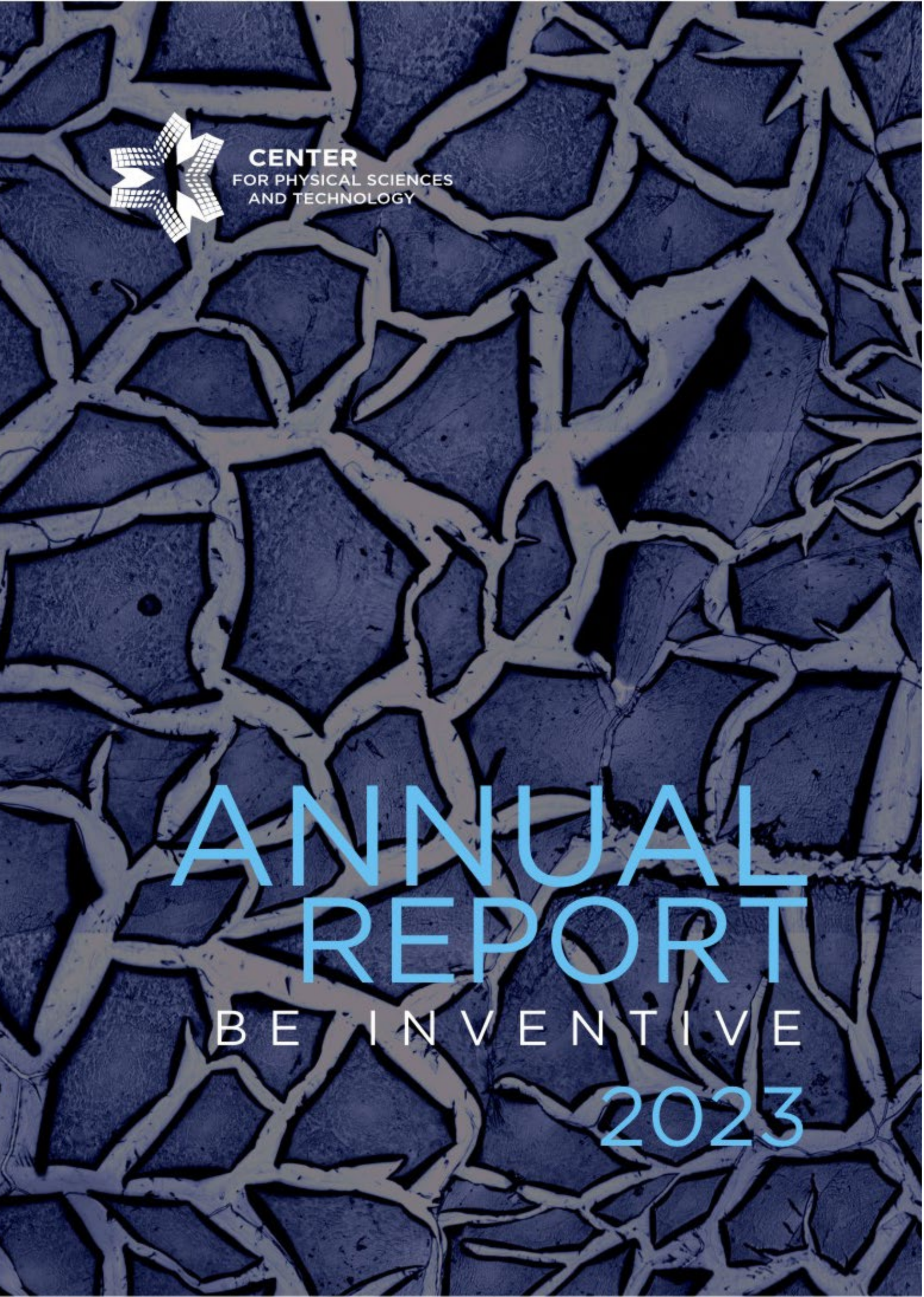

CENTER
FOR PHYSICAL SCIENCES
AND TECHNOLOGY
ANNUAL
REPORT
BE INVENTIVE
2023

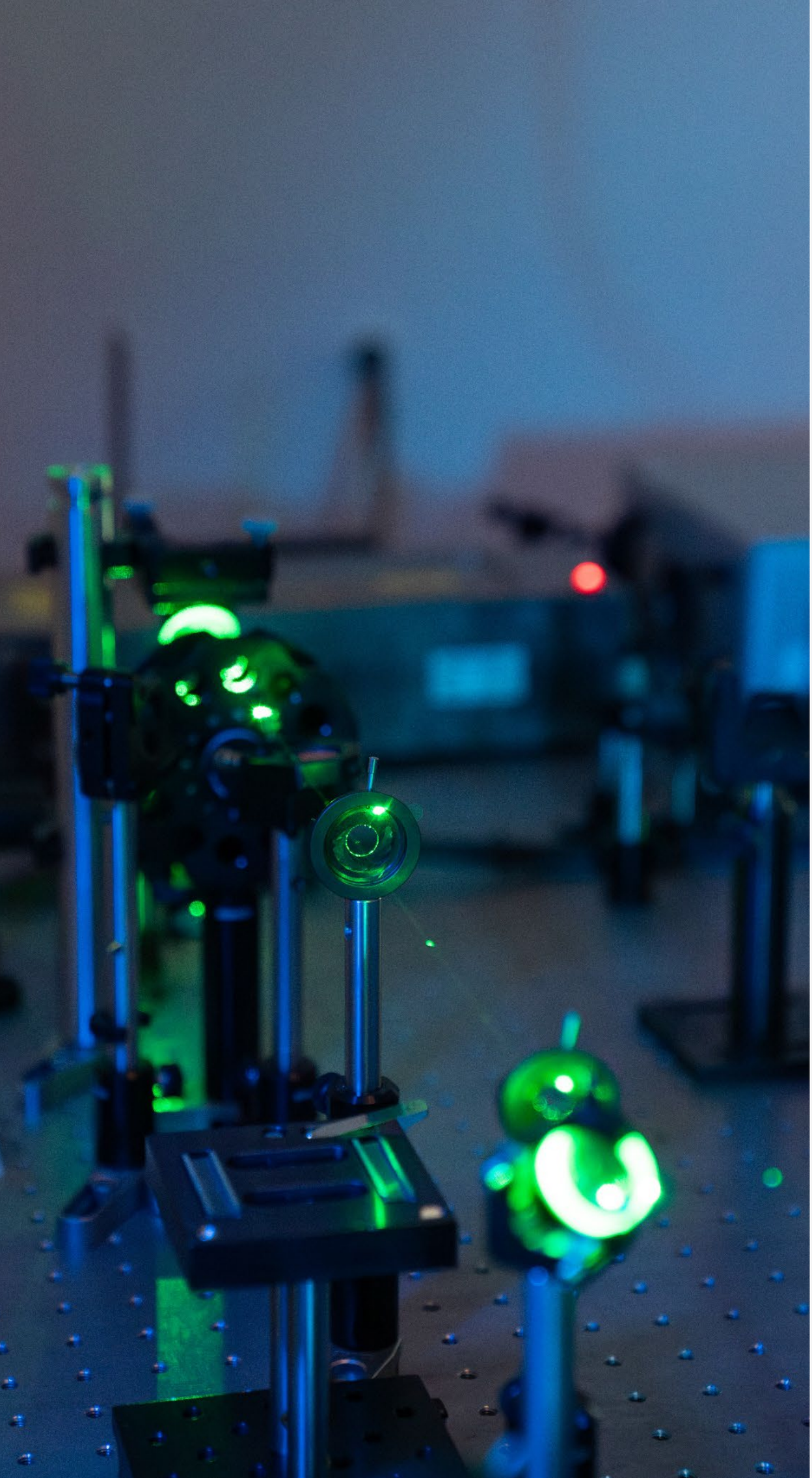



Photo from private archive

Message from Director:

A Year of 2023: Reflections and Extrapolations

The Year of 2023 globally was the year of expanding geopolitical tensions and increased uncertainties, it was the **second year** of Russian invasion to Ukraine. Locally, this has been a year of continual and routine work in advancing knowledge, creating innovations and searching for new discoveries – implementing the results of our laboratories to the market, creating new startups, bridging and expanding connections between high-tech industry and FTMC community.

Despite particular circumstances around and within, **the Year 2023** was an important time for focusing FTMC efforts **to fulfill our mission** – **to generate and capitalize scientific knowledge for the benefit of society and the development of high technologies.**

Our research ideas have continued to contribute to the generation of knowledge and technological development making thus impact at various levels of high-tech innovations. A tremendous efforts were dedicated to extend the grants portfolio from national agencies and councils, private companies, European Commission as well as various overseas funding organizations. It was stimulated by the indications that **scientific, technological and innovation-related activities** of FTMC seems to be approaching the *saturation level*. To encourage our activities, consolidate efforts and experience to increase the number of highly ranked scientific publications, the number of business clients and their contracts in research and development, as well as the number of scientific services, we organized the meetings dedicated to reconsider our scientific topics, technological approaches and attitudes, possible strategic trends and international partnerships.

It is a considerable challenge due to high global competition in these scientific and technological fields. New motto and vision was discussed and accepted: **Be inventive. Our vision is to see FTMC among the best research and technology organisations.**

We believe that FTMC, largest research and technology organization (RTO) in the Baltics, must spread high ambition, strong dedication and professionalism. We think that these features along with our qualifications, united by the streamlined management and a stable strategy based on focused scientific directions, can pave a broad avenue to further achievements – scientific excellence, ground breaking technologies, high-added value innovations and novel smart products or prototypes.

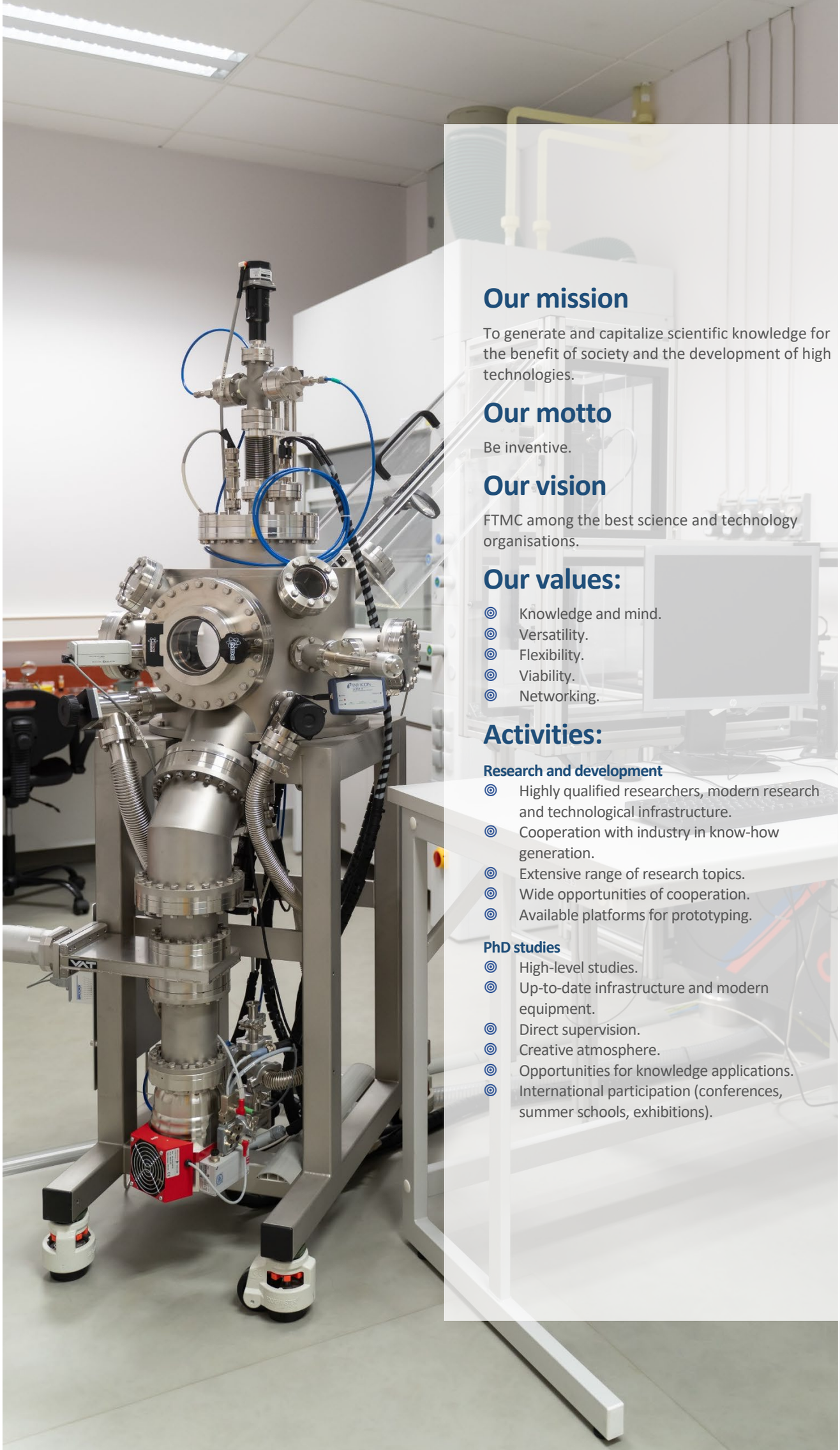
I would like to voice my highest possible appreciation to all the staff members of FTMC, International Advisory Board, our alumni and friends permanently contributing to improvement of our skills and acceleration of FTMC evolution.

I would also like to encourage all of you to increase your efforts into a new qualitative level of the operation mode in the spirit of the FTMC's mission - to be much more effective and much more intensive as still a lot of works are needed to be done.

The **Annual Report 2023** marks an exciting milestone covering the main scientific and technological achievements, as well as the most important events, following us in our mission in a rapidly changing world of technological shaping.

Gintaras Valušis

Vilnius, December 2023



Our mission

To generate and capitalize scientific knowledge for the benefit of society and the development of high technologies.

Our motto

Be inventive.

Our vision

FTMC among the best science and technology organisations.

Our values:

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

Activities:

Research and development

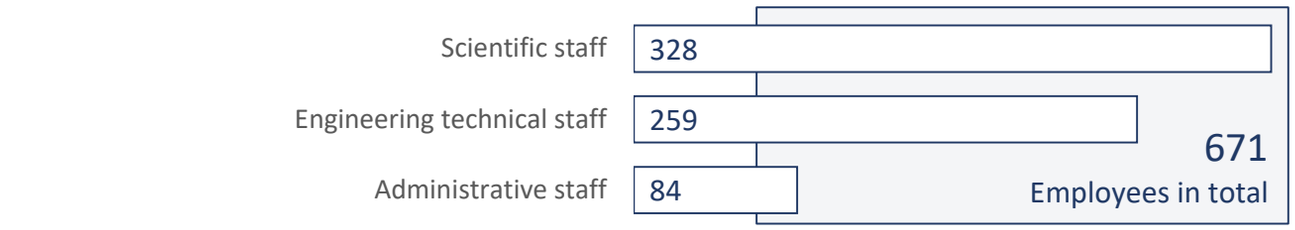
- Highly qualified researchers, modern research and technological infrastructure.
- Cooperation with industry in know-how generation.
- Extensive range of research topics.
- Wide opportunities of cooperation.
- Available platforms for prototyping.

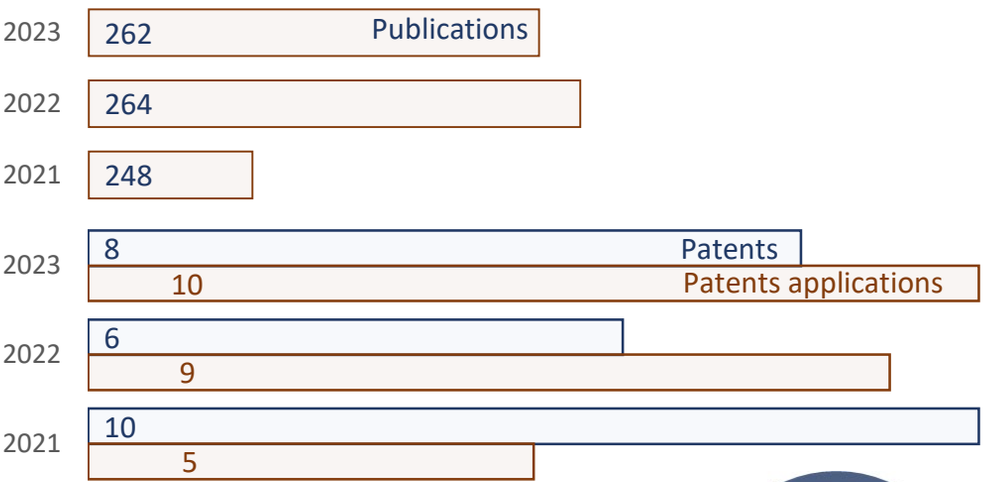
PhD studies

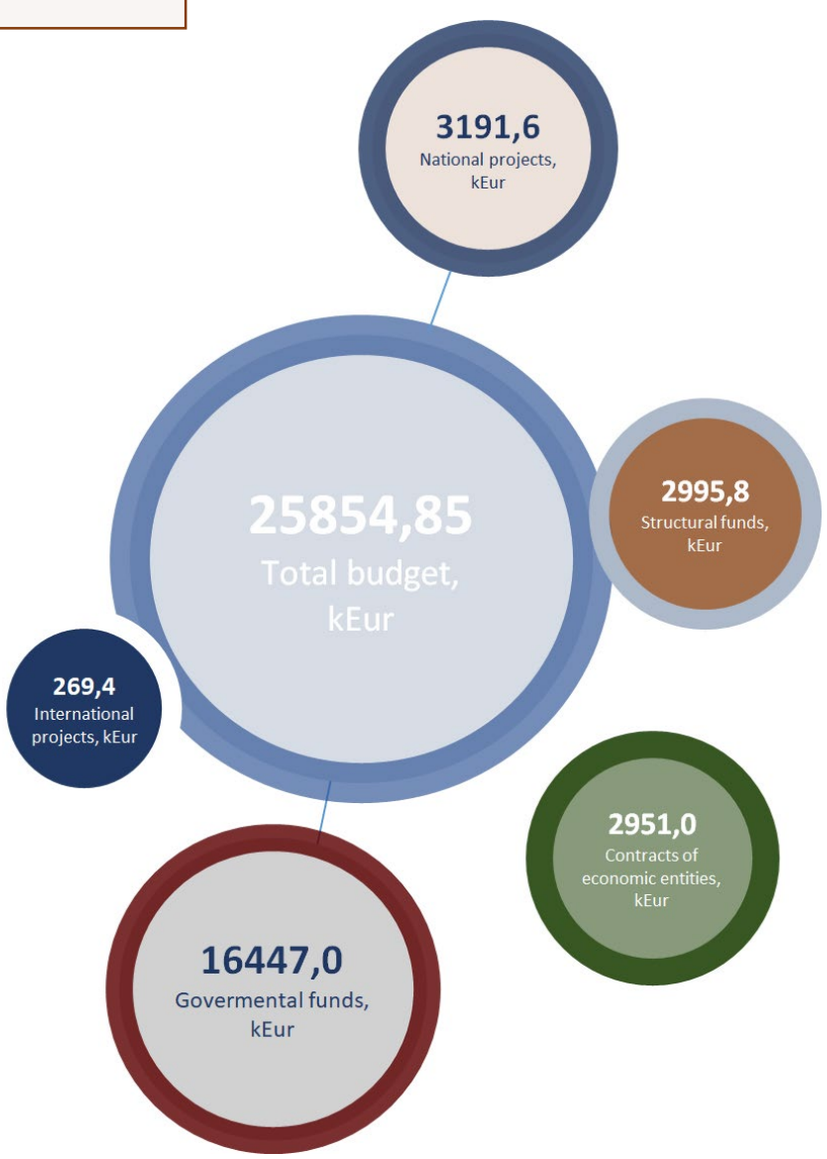
- High-level studies.
- Up-to-date infrastructure and modern equipment.
- Direct supervision.
- Creative atmosphere.
- Opportunities for knowledge applications.
- International participation (conferences, summer schools, exhibitions).

Contents

Facts & figures







Doctoral theses

JEVGENIJ GARANKIN

Development and application of advanced methods based on the application of a polyethylene naphthalate scintillation detector for recording and identification of ionizing radiation. (N 002)
Scientific supervisor: dr. A. Plukis

ROKAS GEGEVIČIUS

Charge carrier transport in hybrid Perovskites. (N 002)
Scientific supervisor: dr. M. Franckevičius

ROKAS JASIŪNAS

Charge carrier generation and extraction in non-fullerene organic solar cells. (N 002)
Scientific supervisor: prof., habil. dr. V. Gulbinas

MAKSIMAS ANBINDERIS

Investigation of detection properties of planar microwave diodes based on A3B5 semiconductor compounds in millimeter–wavelength range. (T 001)
Scientific supervisor: prof., dr. A. Sužiedėlis

JUSTAS DILYS

Research into variability of permanent magnet synchro-nous motor parameters by magnetic field modelling. (T 001)
Scientific supervisors: prof. dr. A. Baškys, prof. dr. V. Stankevič

KIRILL SKOVORODKO

Application of dosimeters and calibrated ionization chambers in optimization of exposure in nuclear medicine procedures. (N 002)
Scientific supervisor: dr. A. Gudelis

EDVINAS NAVAKAUSKAS

The application of sum-frequency generation spectroscopy in studies of biomimetic systems. (N 003)
Scientific supervisor: dr. S. Strazdaitė

RAMAN NOVIKAU

Evaluation of the adsorption properties of composite materials for caesium, cobalt, and europium. (N 003)
Scientific supervisor: dr. G. Lujanienė

SIMONA PŪKIENĖ

Growth and characterization of bismide alloys for infrared sensors. (T 008)
Scientific supervisor: dr. R. Butkutė

LENA GOLUBEWA

Diversiform black silicon for bio-sensing. (N 002)
Scientific supervisor: dr. R. Karpič

KAROLINA MALECKAITĖ

Photophysical properties of boron dipyrromethene (BODIPY)-based fluorescent molecular sensors. (N 002)
Scientific supervisor: dr. A. Vyšniauskas

VITALIY ROMANENKO

The Study of Anthropogenic Radionuclide Transport with Suspended Matter in the System Neman River – Baltic Sea. (N 002)
Scientific supervisor: dr. G. Lujanienė

RUSNĖ IVAŠKEVIČIŪTĖ-POVILAUSKIENĖ

Optical engineering in terahertz imaging and 2D materials inspection. (N 002)
Scientific supervisor: prof., habil. dr. G. Valušis

VINCENTAS MINDAUGAS MAČIULIS

Application of metallic and metal oxides nanostructures for proteins biosensing by ellipsometry and quartz crystal microbalance. (N 003)
Scientific supervisors: prof., habil. dr. A. Ramanavičius, dr. I. Plikusienė

DANIELIUS LINGIS

Numerical simulation of the light ion backscattering spectra in the particle channeling geometry. (N 002)
Scientific supervisor: dr. A. Plukis

PAULIUS GAIGALAS

Synthesis and characterization of effective nanoplatelet structure catalysts for electrochemical water splitting. (N 003)
Scientific supervisor: dr. A. Jagminas

AHMED MOHAMED TAHA ABDELHAMID ALFA

Effects of pulsed electric field on the structural and techno-functional properties of proteins. (N 003)
Scientific supervisor: dr. A. Stirkė

GINTARĖ GEČĖ

Search, synthesis, and investigation of new framework electrode materials for aqueous Na-ion batteries. (N 003)
Scientific supervisor: dr. L. Vilčiauskas

AUDRIUS SADAUNYKAS

Enhancing gas chromatographic analysis: a novel cryo-enrichment module for GC analysis. (N 003)
Scientific supervisor: dr. E. Naujalis

VYTAUTAS ŽUTAUTAS

Applications of conductive polymers in sensors. (N 003)
Scientific supervisor: dr. R. Pauliukaitė

21
New PhD students in 2023

111
PhD students in total

20
Defended doctoral thesis

Main international projects

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
One-Stop-Shop open access to photonics innovation support for a digital Europe – PhotonHub Europe
G. Račiukaitis

Horizon 2020 programme project
Innovation fostering in accelerator science and technology – I.FAST
V. Tomkus

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

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

SPS programme project
3D Metamaterials for Energy Harvesting and Electomagnetic sensing
Ž. Kancleris

Projects partners

UPPSALA
UNIVERSITET

Patents

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

EP 3840050B1
2023-03-29
Natalia Alexeeva, Irmantas Kašalynas

Method relates to the technical field of material science. Method of a polymethylmethacrylate (PMMA) removal from a graphene surface, wherein PMMA layer covers a graphene layer located on a substrate. The method comprises steps as follows: PMMA layer 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 blown with nitrogen to be dried.

System and method for personal thermal comfort

EP 4074206 B1
2023-08-09
Aušra Abraitienė, Diana Kubilienė, Martynas Šapurov, Aldas Dervinis, Vytautas Bleizgys, Algirdas Baškys, Remigijus Bučas

A system for personal thermal comfort comprises a first and a second air blowers, thermoelectric elements, a first heatsink, a second heatsink, an exhaust conduit, one first framework of perforated 3D spacer textile channels for distribution of ambient air flow, one second framework of perforated 3D spacer textile channels for distribution of ambient, extra cooled, or heated air flow, an ambient air distribution valve. The method of modifying a personal microclimate comprises using the first air blower for modification of temperature of the first heatsink, using a second air blower for modification of temperature of the second heatsink, using ambient air distribution valve for controlling ambient air flow to the first framework of perforated 3D spacer textile channels for distribution of ambient air flow for cooling and drying an area of a user's body, and to the second framework of perforated 3D spacer textile channels for distribution of ambient, extra cooled, or heated air flow for further cooling, extra cooling or heating an area of a user's body.

Method for formation of the diffractive optical element consisting of plurality surface microstructures

LT 6983 B
2023-03-10
Evaldas Stankevičius

Method for formation of the diffractive optical element consisting of plurality surface microstructuresABSTRACTThe invention relates to the formation of diffractive optical elements in a photopolymer, where the formed elements can be used in the splitting of a light beam. The polymeric diffractive optical element is formed by treating the photopolymer layer with a defocused femtosecond laser beam, and the diameter of the affected spot is ≤20µm. In the laser exposed area of the photopolymer, a photopolymerization reaction is initiated, which makes the affected area insoluble in an organic solvent. By scanning the laser beam in the photopolymer, an array of microstructures is formed. The inner arrangement of microstructures determines the diffractive properties of the optical element. The optical element can also be used as a generator of the Bessel-type beam array in the near field.

Method of manufacturing an electrochemical cell and an electrochemical cell

LT 7025 B
2023-09-25
Arūnas Ramanavičius, Simonas Ramanavičius, Urtė Prentice, Linas Sinkevičius, Almira Ramanavičienė

A method of manufacturing an electrochemical cell and an electrochemical cell so obtained is disclosed. The method comprises providing a multi-layered ceramic-metal capacitor, removing insulating coating at a side area of the capacitor to expose side edges of ceramic dielectric material and metallic plates of electrodes. The opening is covered with insulating material so that terminals of the electrodes could be coated with insulating material. The cover of the opening is removed and edges of plates of the electrodes are functionalised by electrochemical plating. The terminals of the electrodes are connected to signal transmitting means for transmitting signals from the electrodes. One or more pairs of such electrodes are obtained in such way to form a multi-electrode electrochemical system. Electrode system can be placed in any type of electrochemical cells including designing of multiple electrochemical cells within multi-wailed) plates of enzyme linked immune sorbent assay (ELISA)-plate or similar multi-wailed systems.

The laser radiation transforming device used for the laser processing of materials

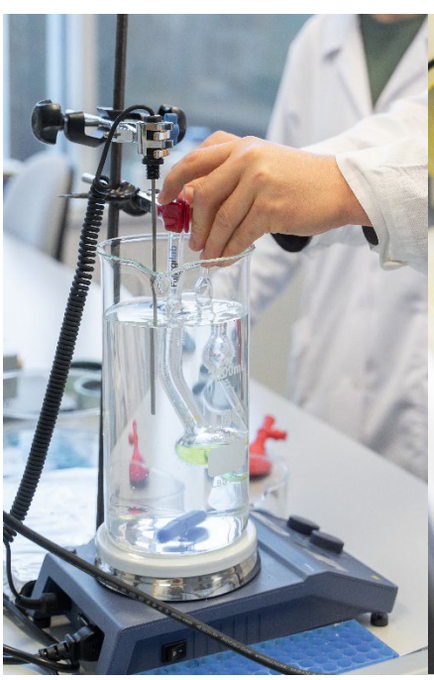
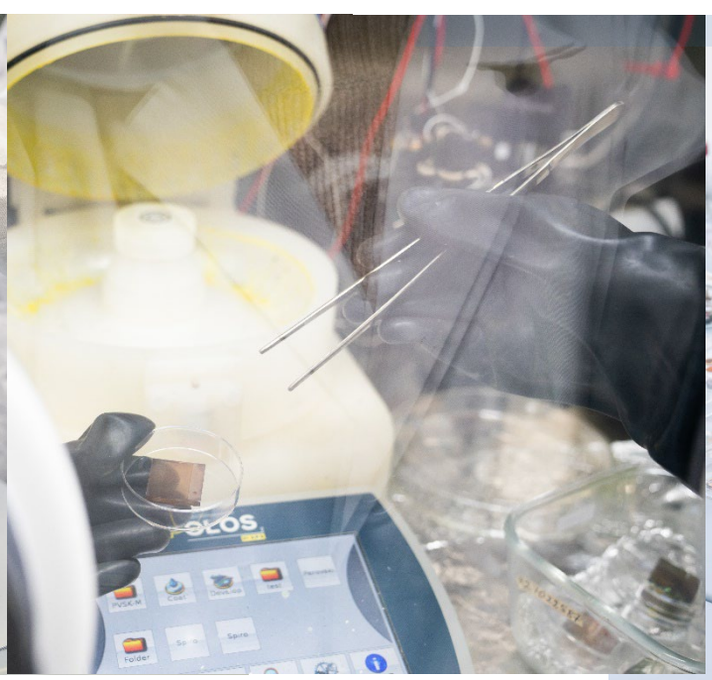
LT 7027 B
2023-09-25
Sergejus Orlovas

The invention belongs to the field of material processing and relates to the use of laser light to remove material from a workpiece and can be applied to the processing of transparent media, including glass. The laser radiation transforming device has a photonic element consisting of a transparent material base, the input and output planes which are arranged parallel to each other. There is a structural modification in the base volume of the transparent material between the input and output planes of the photonic element or at the surface of the photonic element. The structures recorded in or on a photonic element are geometric Pancharatnam-Berry phase structures with uniformly varying angles of their orientation, which at each point of the beam cross-section gives the change function of the orientation of the structures $\vartheta = f(\varphi, r)$, where φ is the azimuthal angle of the element's coordinates, varying from $-\pi$ to π, and r is the radial coordinate. The polarization angle change function $\vartheta = f(\varphi, r)$ is created in such an oscillating form that when the radiation exiting from the photonic element is focused, a photonic needle of the desired shape is formed, regardless of the polarization direction of the incident light field.

Method and apparatus for shaping a light pulse

LT 6971 B
2023-01-10
Kęstutis Regelskis

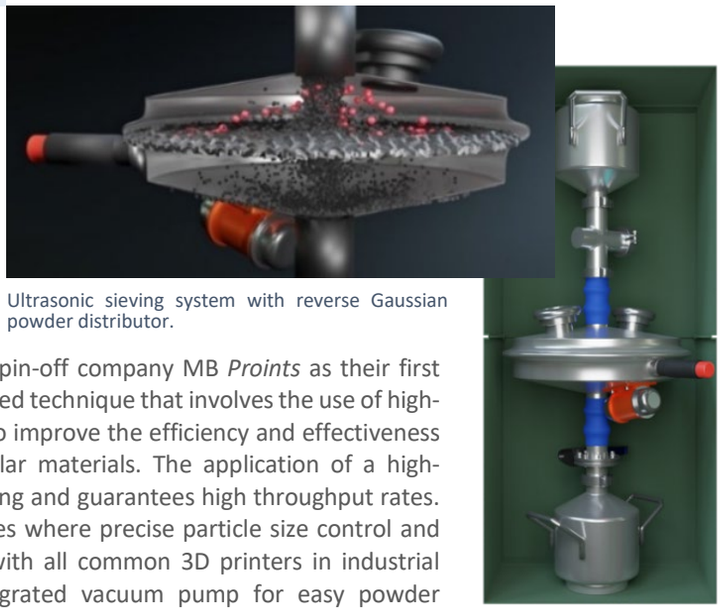
Method and apparatus for shaping a light pulseABSTRACTThe invention relates to the field of laser technology and is intended for a regenerative method and device for shaping a light pulse determined by the parameters of the regenerative circuit (DPRC) from an initial light pulse. An initial light pulse is injected into a regenerative circuit, where a DPRC light pulse is shaped with a specified precision and then output. In order to improve the accuracy of the shaped light pulse for the given parameters while simplifying the device, the light pulse is shaped by regenerating it in the same regeneration circuit, which is closed by the controlled optical switch until the DPRC light pulse is shaped with the specified accuracy, or up to a predetermined number of roundtrips, or in advance a certain period of time during which the DPRC light pulse is shaped from the initial light pulse with a predetermined precision, which is outputted from said regenerative circuit, and the regenerative circuit is disconnected before the next initial light pulse is input. The invention relates to the field of laser technology and is intended for a regenerative method and device for shaping a light pulse determined by the parameters of the regenerative circuit (DPRC) from an initial light pulse. An initial light pulse is injected into a regenerative circuit, where a DPRC light pulse is shaped with a specified precision and then output. In order to improve the accuracy of the shaped light pulse for the given parameters while simplifying the device, the light pulse is shaped by regenerating it in the same regeneration circuit, which is closed by the controlled optical switch until the DPRC light pulse is shaped with the specified accuracy, or up to a predetermined number of roundtrips, or in advance a certain period of time during which the DPRC light pulse is shaped from the initial light pulse with a predetermined precision, which is outputted from said regenerative circuit, and the regenerative circuit is disconnected before the next initial light pulse is input. The invention relates to the field of laser technology and is intended for a regenerative method and device for shaping a light pulse determined by the parameters of the regenerative circuit (DPRC) from an initial light pulse. An initial light pulse is injected into a regenerative circuit, where a DPRC light pulse is shaped with a specified precision and then output. In order to improve the accuracy of the shaped light pulse for the given parameters while simplifying the device, the light pulse is shaped by regenerating it in the same regeneration circuit, which is closed by the controlled optical switch until the DPRC light pulse is shaped with the specified accuracy, or up to a predetermined number of roundtrips, or in advance a certain period of time during which the DPRC light pulse is shaped from the initial light pulse with a predetermined precision, which is outputted from said regenerative circuit, and the regenerative circuit is disconnected before the next initial light pulse is input.


Prototypes

Ultrasonic powder sieving for industrial additive manufacturing

genrik.mordas@ftmc.lt



Ultrasonic sieving system with reverse Gaussian powder distributor.

The researchers at FTMC Laboratory of 3D Techno-logies and Robotics, using the Laser-Powder Bed Fusion technology, developed the ultrasonic powder sieving system with a reverse Gaussian powder distributor, which facilitates time-consuming pre-processing. The unique patent-pending technology is commercialised by a spin-off company MB *Proints* as their first product, SEPA. Ultrasonic powder sieving is a specialised technique that involves the use of high-frequency (18 kHz and higher) ultrasonic vibrations to improve the efficiency and effectiveness of the sieving process for fine powders and granular materials. The application of a high-frequency ultrasonic vibration prevents screen clogging and guarantees high throughput rates. Ultrasonic powder screening is beneficial in industries where precise particle size control and product quality are essential. The machine works with all common 3D printers in industrial additive manufacturing. The machine has an integrated vacuum pump for easy powder transportation and allows for wide variation of sieves (from 20 to 200 µm). Powder handling is operated intuitively via the touch panel. The system works fully automatically via recipes and achieves a sieving capacity of up to 30 litres per hour.

The way to new functional design

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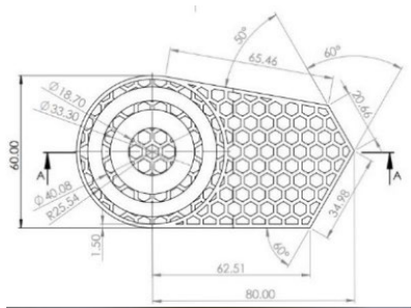
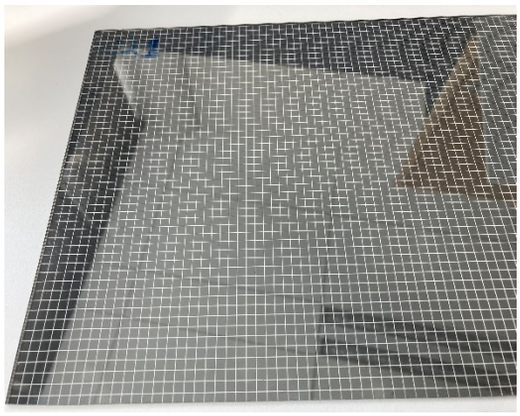
karolis.ratautas@ftmc.lt

The modern automotive industry is constantly looking for new technological solutions to improve the design, functionality and efficiency of cars. One of these innovative solutions is to combine two technologies: additive manufacturing and laser-chemical technology of selective metal deposition, known as Selective Surface Activation Induced by Laser (SSAIL). The combination of these two technologies offers many advantages - it fundamentally transforms conventional production processes and provides exceptional freedom for shapes and designs. We realised those ideas and developed a functional car LED lamp. It could complement the design of the modern car and improve the lamp's efficiency and lifetime.



Drawing and prototype of a functional car LED lamp.



Low-emission glass with IR reflective thin metal coating and laser texture.

Textures on low-emission glasses for mobile communication

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Low-emission window glasses contain thin metal films to reduce thermal energy losses through windows. However, this significantly reduces the transmission of microwaves used in mobile and wireless communication. The research was carried out on glasses with metallic coatings to achieve selective transmission of electro-magnetic waves at the frequencies of mobile phones. Textures of various shapes on the glass metal coating were modeled and optimal geometries were selected. The optimal textures were realised on low-emission glass prototypes with a metallic coating. The texture ensures enhanced transmission of microwaves at the frequency bands of 1800 MHz, 2100 MHz, 2600 MHz and 3500 MHz for mobile telecommunication.

Embedded Fresnel optics

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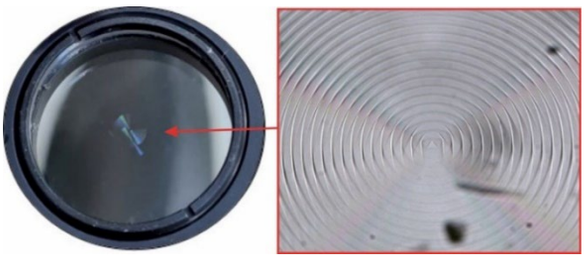
The research at the LATEKOC project was carried out in the volume modification of glass. Irradiation with a focused beam of femtosecond laser led to a refraction index modulation of the material permitting manipulation of the light properties. A demonstrator of the fraxicon, a light-forming optical element, was produced and verified.



Demonstrator of the fraxicon recorded in the volume of UVFS glass by laser writing technology.

Demonstrator of the fraxicon recorded in the volume of UVFS glass by laser writing technology.

Laser-made microlenses

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The milling technology of glass subtractive processing was developed, based on milling of 2.5D surfaces with laser radiation. After laser milling, the surface roughness can reach Ra=0.8-0.3 µm. An additional CO_2 laser polishing technology was applied to make surfaces of optical quality. The surface roughness was reduced by more than 16 times after the polishing process. Both plano-convex lens and arrays of microlenses were formed using the combined technology.

Smart window prototype

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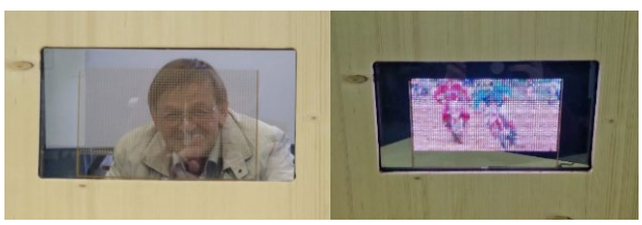
By combining the newly developed technologies of subtractive laser processing for inorganic dielectric and laser-induced selective metal deposition, a smart window prototype was produced as a part of the LATEKOC project activities. The smart window prototype consists of:



Smart window prototype.

- Low-emission glass with a thin metal coating in which a resonant grid is formed by a laser to improve by 2 times radio wave transmission at 2 GHz radio frequency;
- Glass with integrated interactive LED display with metal interconnections made by the selective laser-assisted metal deposition with assembled mini-LEDs and other discrete electronic components.

Wireless system to control the cleanliness of a food production conveyor

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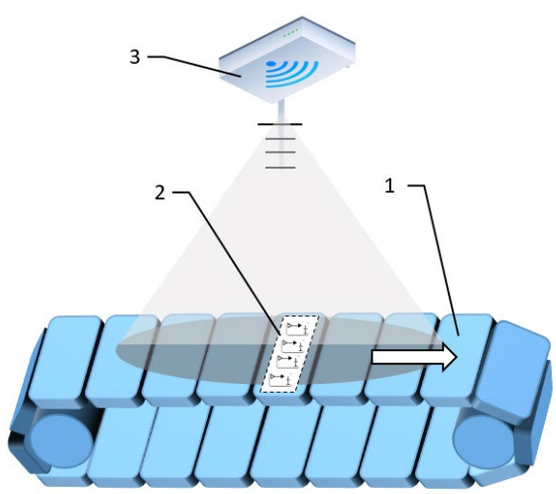
romualdas.trusovas@ftmc.lt



Schematic view of a wireless food production conveyor cleanliness control system: 1 – the ordinary segment of the conveyor, 2 – the segment with a pH sensor and antennas, 3 – the WiFi hub.

The system to control the cleanliness of a conveyor consists of a pH sensor, which controls the use of disinfection means and is an indicator of the cleanliness of the conveyor, a measurement and data transmission unit, and a microwave antenna unit that ensures connection with an external router and microwave energy harvesting to power the control system installed on the moving part of the conveyor. The control system was developed as a part of the SMART project BEGAMA in collaboration of researchers from three FTMC departments. The Laser Technologies Department has developed a system, collecting sensor readings and transmitting them to the router, and applied the SSAIL technology for the manufacturing of microwave antennas and pH sensor contacts. The Microwave Laboratory at the Department of Physical Technologies has developed a wireless system for the harvesting of microwave energy. The Department of Nanoengineering has developed a pH-sensor that monitors the cleanliness of the conveyor's surface. The developed control system was validated under laboratory conditions.

Awards

Evelina Dudutienė

breakthrough junior challenge –
for her excellent PhD thesis awarded as one of the best PhD works of the Year 2022 in Lithuania; for her enthusiasm and passion in building young researchers' team oriented to optical investigation of semiconductor nano-structures.

Jurga Juodkazytė

for scientific achievements –
for widely recognized scientific works in photo-electronchemistry and permanent search of their implementations.

Rimantas Ramanauskas

for life achievements –
for the tremendous scientific input in the field of chemistry and permanent care on the development of chemical technologies at FTMC.

Vidmantas Remeikis

for life achievements –
for the widely recognized scientific achievements in nuclear physics and the establishment of the FTMC.

Tadas Paulauskas

for innovations –
for fruitful versatile activities in initiating topic on quantum technologies and related encouraging experimental and theoretical investigations.

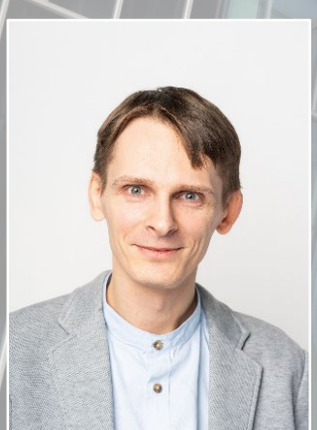
Lukas Razinkovas

Irena Grybienė

for scientifically invisible activity –
for long-standing patient and precise work at the Maintenance department.

Marija Gutauskienė

for scientifically invisible activity –
for sincere and large scale activities decorated with responsibility, professionalism and lovely atmosphere.



Simonas Bendžius

recipient of the special award –
for renesanse of public relations, for his inexhaustible energy in preparing attractive highlights on FTMC scientific achievements and illuminating Podcast "So what are you doing there?"

Events

2023.01.26

The lawyer, investor and philanthropist Marius Jakulis Jason was awarded the FTMC Patron Sign

for Marius Jakulis Jason (MJJ) Foundation research grants to three scientists, who came back to FTMC from foreign scientific institutions (dr. A. Baradokė, dr. V. Žičkus and dr. E. Auksorius), and the foreign researcher K.N. Alekseev, who was recruited to FTMC staff.

2023.02.16

Kęstutis Pyragas was awarded the Officer's Cross of the Order of Grand Duke Gediminas of Lithuania

The President of Lithuania awarded the Officer's Cross of the Order of the Grand Duke Gediminas of Lithuania to Kęstutis Pyragas - physicist, professor, habilitated doctor for his significant contribution to the development of physics and for his world-class achievements. K.Pyragas is the head of the Laboratory of Nonlinear Dynamics and Nanophysics of the Fundamental Research Department of FTMC. His contribution to chaos theory is extremely important (one of the chaos management algorithms is called the Pyragas method), and the scientific article written in 1992 remains the most cited work of Lithuanian physicists.

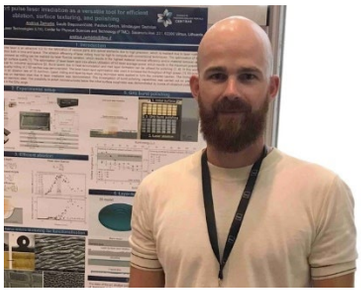
2023.02.23

Director of the FTMC, academician, prof. Gintaras Valušis celebrated his 60th birthday

On this special occasion, the FTMC Science Council and administration, representatives of the Parliament, the Ministry of Education, Science and Sports, the Academy of Sciences, Vilnius University, colleagues and friends congratulated the respected scientist and leader of the FTMC community. G. Valušis is a widely known semiconductor physicist working in the terahertz field. He has published more than 275 scientific articles widely cited by the international community, and was awarded the Lithuanian Science Prize. He dedicated a large part of his scientific career to the implementation of the Sunrise Valley project, thanks to which, now most of the FTMC community works in one building, and the FTMC has become internationally well-known institution.

2023.02.24

Dr. Andrius Žemaitis became the laureate of the LMA Young Scientists and Doctoral Students Award



The researcher of FTMC Laser Technologies Department dr. Andrius Žemaitis was awarded a prize, established by the Lithuanian Academy of Sciences (LMA) for young scientists and doctoral students in the field of mathematics, physics and chemistry, for his work "Laser processing with ultrashort pulses: optimization and applications".

2023.03.09

Dr. S. Ramanavičius received *Polymers* journal award for the best doctoral thesis in 2022

FTMC researcher was recognized for his work related to the development of new nanomaterials (titanium suboxides and MXenes, the two-dimensional nanostructures discovered in 2011 and currently receiving a lot of attention). He was looking for ways to more efficient formation of the studied nanomaterials, as well as for controlling their properties during synthesis, in order to use them in practice as sensors for recognizing various gases or drug fragments.

2023.03.22

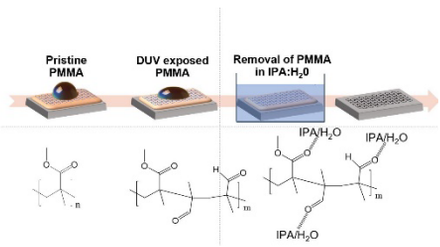
A Lithuanian professor from FTMC published a book that is read all over the world

Our colleague, Prof. Hab. Dr. **Eimutis Juzeliūnas**, world-renowned electrochemist, laureate of the Lithuanian Science Prize, at the end of 2022 published the book *Silicon: Electrochemistry, Production, Purification and Applications* (ed. Viley-VCH), which enriches our knowledge about silicon. There are only a few monographs on silicon electrochemistry worldwide, and the last one was written 20 years ago.

2023.03.23

ELI - laser particle accelerators, their applications, and possibilities of experiments

The Extreme Light Infrastructure (ELI) workshop took place at FTMC, where laser technology specialists from the Czech Republic, Hungary, France, Germany, Italy, Spain and Lithuania were gathered. ELI is an international laboratory system that uses high-power lasers. Their creation and development is supported by the European Strategy Forum on Research Infrastructures (ESFRI). ELIs are powerful ultrashort pulse lasers that produce high radiation intensity. They make it possible to study new phenomena using accelerated electric particles, electrons and protons. The particles accelerated by a powerful laser can then be used for diagnostics, materials research, and radiotherapy. One of the areas is new cancer treatment technologies. Some of the ELI laser components are made by Lithuanian companies Light Conversion and Ekspla.



2023.03.29

Unique invention: ecological way of purifying graphene

FTMC scientists Natalia Alexeeva and Irmantas Kašalynas were the first in the world to patent an ecological way of purifying graphene. The European Patent Office issued the patent *Method of polymethylmethacrylate (PMMA) removal from a graphene surface by photoexposure*. The invention of these two scientists is the first in Europe and the world. An offer has been received to extend this patent to the US, Japanese and Chinese markets. The obtained patent also means that FTMC has the first right in Europe to use such technology in production, to license and sell it. The Innovation Service of FTMC is looking for ways to get business interested in the new method.

2023.04.04

Arūnas Krotkus - 75

Leading researcher of the FTMC Optoelectronics Department, academician, Lithuanian Science Prize laureate, prof. Hab. dr. Arūnas Krotkus celebrated his 75th birthday. All of us wished him strong health and creative energy. We wished that his curiosity and intuition of a researcher, thanks to which he managed to beat time and still inspire us with the charms of physics, would never end.

2023.04.18 – 2023.04.21

The International conference for students OPEN READINGS 2023

The 66th international conference for students of Physics and Natural sciences OPEN READINGS 2023, was held at FTMC, most advanced institution for physical, chemical sciences and technology in Baltic States. More than 350 participants from various countries took part in the conference. Young scientists presented their research in thirteen areas of natural sciences and technologies. Participants and listeners had the opportunity to attend the lectures of guest lecturers. World-renowned scientists shared their knowledge in the fields of quantum optomechanics, epidemiology, organic optoelectronics, astrophysics, lasers and more.

2023.04.26

FTMC was visited by the Science Director of the Naval Research Office of the US Defense Department

Martina Barnas, the science director of the Naval Research Office of the US Defense Department visited the Textile Technology Department of FTMC in Kaunas, accompanied by Andrea Lindgren, the official of the US Embassy in Lithuania supervising scientific issues in the Baltic region. The guests were interested in textile technologies developed in Lithuania and discussed the opportunities for cooperation of FTMC with research institutions in the USA.

2023.05.09

A team of FTMC scientists developed a unique metal lens

A group of FTMC researchers (R. Ivaškevičiūtė-Povilauskienė, V. Čižas, E. Nacius, I. Grigelionis, K. Redeckas, M. Bernatonis, S. Orlovas, G. Valušis and L. Minkevičius) has published an article in the high-profile international journal Frontiers in Physics on the development of thin metal lens. It is designed to improve and simplify terahertz imaging, the process of scanning an object with invisible terahertz rays to produce one or another visible image.

2023.05.15

Famous physicist Audrius Alkauskas died at the age of 45

Leading scientific researcher of Fundamental Research Department of FTMC dr. A. Alkauskas was an active and productive scientist who left his trace in various fields - from optoelectronics to quantum physics. He was also known and appreciated in the public sphere for his intelligence and ability to explain complex matters by simple and visual language. He was nominated in the LRT 2020 Awards in the Discovery of the Year nomination for determining the nature of quantum emitters in two-dimensional semiconductors. From 2002 to 2010, Audrius lived in Switzerland, where he defended his doctoral thesis and worked as a postdoc. In 2011-2014 A. Alkauskas was a researcher at the University of California in Santa Barbara. Since 2014 he lived in Vilnius. The areas of scientific activity of A. Alkauskas were material science, solid state, surface, interfaces and defects physics, density functional theory, physics of renewable energy sources and solid-state theoretical spectroscopy. Like a comet, he was so bright, but lived so shortly. All our community will truly miss him.

2023.06.13

The Lithuanian Army signed the cooperation agreements with FTMC

With this document, the parties undertake for at least one year to cooperate in educating and informing the public about Lithuania's security and defense policy, the Lithuanian Army and its role in ensuring the country's security, developing civil society and its awareness, and introducing innovations in the field of defense. Commander of the Army Training and Doctrine Board Brig. Gen. Alvydas Šiuparis emphasized the need for unity and thanked new colleagues for their serious approach to national defense and understanding of the geopolitical situation and challenges of Lithuania.

2023.07.04

Chemist-engineer Svajus Asadauskas died at the age of 56

S. Asadauskas worked in the Department of Chemical Engineering and Technology of FTMC as a Leading Researcher and Head of the Tribology Laboratory. We have lost one of the most famous Lithuanian tribologists. S. Asadauskas studied chemical technology at the Kaunas University of Technology. In 1993, he went for PHD studies to Pennsylvania State University (USA), where defended his doctorate in chemical engineering in 1997. For three years, S. Asadauskas worked at the US Department of Agriculture, where he researched how oil could be replaced by vegetable oils in the production of lubricants. Later, S. Asadauskas changed his civil service to work in the US branch of the German company Fuchs Lubricants, where he worked for eight years. In 2008, he returned to Lithuania. Our community will greatly miss an always cheerful and sincere colleague, whose advice and insights were useful not only in the scientific field.

2023.08.31

FTMC researchers will participate in a new international project funded by the European Defense Fund

The researchers of the Departments of Textile Technology and Physical Technology of the FTMC received good news: the financing of a new European Defense Fund program project ACROSS (Adaptive Camouflage for soldiers and vehicles) has been approved. This project is aimed at improving the existing technologies for creating adaptive camouflage of land systems (military and transport platforms), using innovative materials and aiming to create camouflage systems that ensure protection in wide spectrum of ranges (UV, visible, IR, radar radiation). Eighteen partners from nine European countries will participate in this project.

2023.09.19

Two representatives of FTMC are among the winners of Young Scientists Scholarship competition of the Lithuanian Academy of Sciences

Physicist from Laser Technology Department dr. Paulius Mackonis was awarded for the research *Development of advanced high-intensity mid-infrared laser architectures*. He was honored for the most important achievements of recent years in the generation and amplification of ultrashort laser pulses in the mid-infrared (IR) spectral region. A researcher at the Department of Electrochemical Materials Science dr. Simonas Ramanavičius, was awarded for his work *Application of 2D MXen nanostructures for the detection of biomolecules using surface-enhanced Raman spectroscopy*, in which he presented a method of the specific molecules recognition.

2023.09.22

FTMC team has won the Startup Pitch Battle

PhD students Kasparas Kižys, Pamela Rivera and Romuald Petkevič received an investment of €125,000 from the early-stage VC fund Baltic Sandbox Ventures focused on fostering the lifesciences and deeptech ecosystem in the Baltics. The investment comes with an invitation for the startup to join a tailor-made acceleration program which helps to advance in commercialization of technology and expand to international markets. Team's idea is to "recruit" yeast to generate electricity by eating our wastewater. FTMC sees a huge applicability of this project in agriculture and wastewater management for individual homes. It is expected to replace thermal power plants in future.

2023.10.18 – 2023.10.19

Conference of Doctoral Students and Young Researchers FizTech2023

The 13th conference of Doctoral Students and Young Researchers FizTech2023 was held at FTMC. The current research, obtained results and their possible applications were presented by the Doctoral students of Physics, Chemistry, Material engineering and Electrical and electronic engineering.

2023.10.18

Raimonda Bogužaitė, the creator of molecular fingerprints, won the X Factor for Lithuanian scientists

More than 100 years ago, police investigators began using fingerprints to track down criminals. Today, chemists are developing molecular fingerprints to help sensors track viruses and other wanted objects. R. Bogužaitė, a PhD student of the Department of Nanotechnologies of FTMC, won the researchers Grand Prix 2023, a unique competition for young scientists in Lithuania. She presented a topic about development of electrochemical sensor based on modification of polypyrrole properties. She and her colleagues are looking for solutions to develop a sensor based on molecular imprinting technology.

2023.11.22

Quantum Technologies Association of Lithuania was founded

The Association brings together FTMC, Vilnius University and the information technology company Novian Technologies. As it was told by the head of Association dr. Tadas Paulauskas, there are well-known physicists from Physics Faculty of Vilnius University involved in technological development as well as a group of mathematicians and computer scientists of Vilnius University who, together with their foreign colleagues, are developing quantum algorithms and testing them on quantum computers. At FTMC, quantum systems of particular relevance to technology have been the subject of theoretical research (and considerable collaboration with experimental workers) by the team of dr. Lukas Razinkovas. As the business is interested in quantum technologies as well, the collaboration of scientists and businessmen is important to find solutions for technologies developed in laboratories to be transferred into products.

2023.11.29

Agnė Zdaniauskienė - the author of the best PhD thesis in 2022

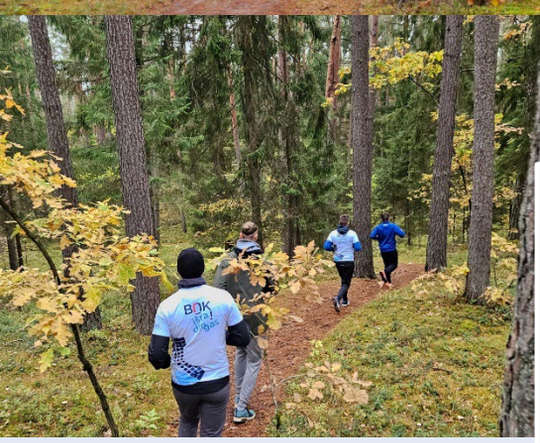
In the contest of theses organized by the Union of Young Scientists of Lithuania, the researcher of the Organic Chemistry Department of FTMC, dr. **Agnė Zdaniauskienė** was announced the winner in the research field comprising the nature, technology, medicine and health and agricultural sciences for the dissertation entitled "*Characterization of biomolecules by nanoparticles, covered with a protective layer, by enhanced Raman spectroscopy*". Another thesis of the FTMC researcher was among the top five. The physicist of the Optoelectronics Department, dr. **Evelina Dudutienė**, received the award for the work "*Photoluminescence properties of GaAsBi quantum holes and Bi quantum dots*".

2023.12.22

The new material to boost the efficiency limits of silicon solar cells

A research group from FTMC together with partners from Tallinn University of Technology (Estonia) set out to synthesize new material that could potentially complement the silicon solar cell technologies and increase the overall efficiency of the solar modules.

Beyond science



A new tradition: FTMC Fall Cross Country Running in Aukštagiris Forest.

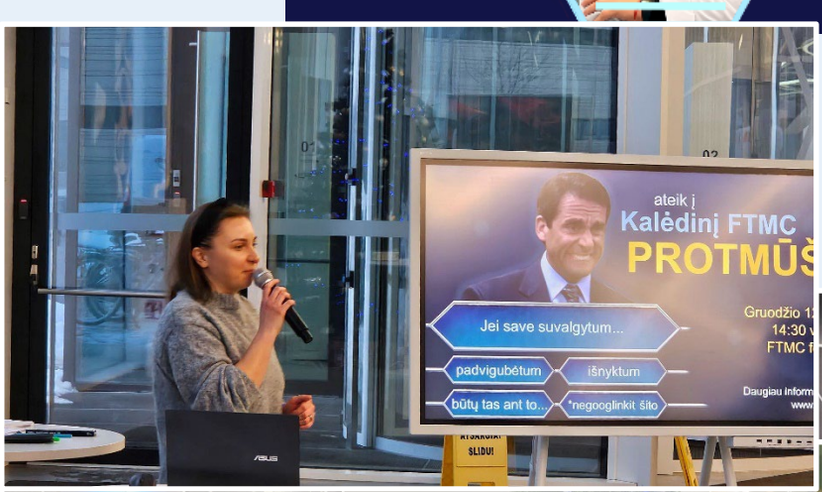
PhD student Yaraslau Padrez performed well in the marathon "Vilniaus tiltai" and took 3rd place among 104 participants in the half-marathon race!

National Mobility Challenge: FTMC scored the highest step average in the "High School" category!

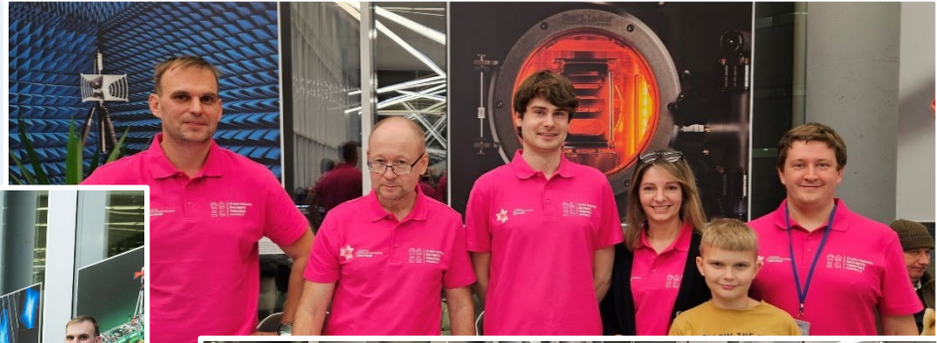
- FTMC hosted the first Maltese hackathon for children and youth.

- FTMC scientist dr. Ieva Plikusienė was chosen European of the Year, in the category "For promoting the name of Vilnius in Europe".

- FTMC launched the science popularization podcast "So what are you doing there?".

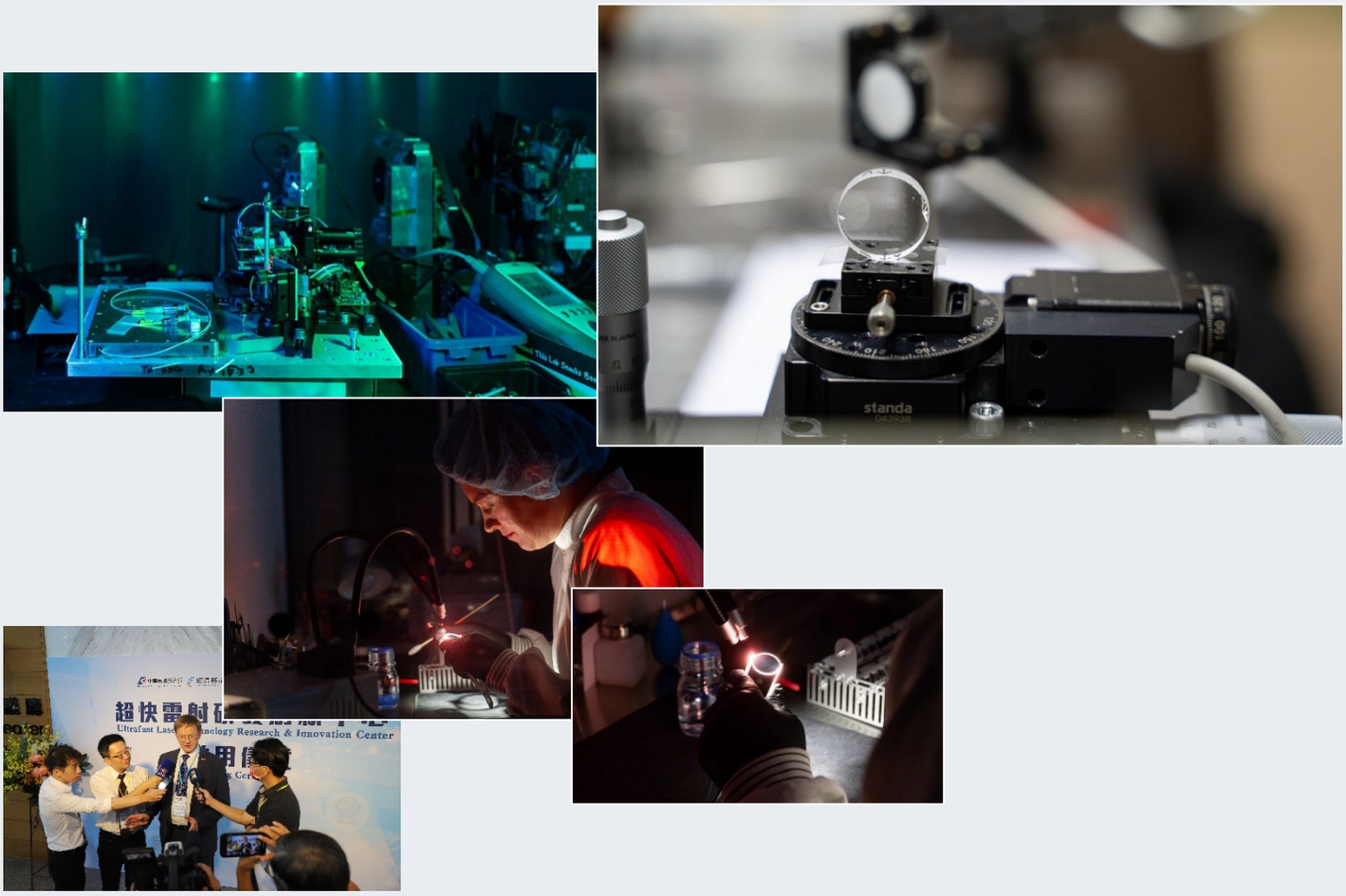


- A Christmas brainstorming session where teams competed to answer questions about science, history, jokes, music and of course Christmas.



◎ The 4th FTMC Chess Tournament.

◎ Traditional Christmas fair organized by „Laisvalaikio laboratorija”



Department of Laser Technologies

Dr. Gediminas Račiukaitis
Head of Department,
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The Department of Laser Technologies focuses its research on optics, lasers and laser technologies. 2023 was another busy and successful year for us. We completed the implementation of the Competence Centre project LATEKOC to demonstrate additive and subtractive laser technologies for the production of integrated electronics on free-form inorganic dielectrics. A few SMART projects: LAFREZA, BEGAMA were dedicated to the development and application of laser technologies; LASERCOM on lasers for space-to-ground communication and ULTRABRAIN on new laser sources for multiphoton microscopy, providing new opportunities for neuroscientists to study the progression of Alzheimer disease.

Our activities were continued in H2020 projects Multiscan 3D and i.FAST. The interaction of ultra-intensive laser beams with gas targets, leading to laser wakefield acceleration and X-ray generation, was intensively studied collaborating with researchers from leading European laser facilities, including ELI – Extreme Light Infrastructure. The department is deeply involved in the Digital Innovation Hub (DIH) network, participating in pan-European laser- and photonics-specialised DIHs PhotonHUB Europe and PULSATE, as well as the regional EDIH.LT, providing test-before-invest support to local companies. Laser-based advanced and additive manufacturing technologies are seen as one of the key enablers of digital manufacturing. 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. Establishing the Ultrafast Laser Technology Research and Innovation Center (ULTRI) at the Industrial Technology Research Institute (ITRI) in Taiwan was a significant step in the internationalisation of FTMC and our department activities. New research and knowledge transfer opportunities have been opened in collaborating with Taiwanese universities, ROTs and companies.

High-efficiency BiBO-based optical parametric chirped pulse amplifier with ~2.2 mJ, 38 fs output at ~2.2 µm

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The compact and cost-effective high-intensity mid-IR laser system demonstrated an unprecedented ~25% efficiency. A Yb:YAG laser provided >10 mJ, 1.2 ps pulses at 1030 nm to pump a three-stage optical parametric chirped pulse amplifier (OPCPA) based on BiBO crystals and to drive the supercontinuum seed. The energy of amplified pulses in the wavelength range 1.95–2.4 µm reached ~2.2 mJ and after compression a pulse duration of 38 fs was obtained. The laser system makes it possible to achieve high efficiency of THz generation and higher energy of X-ray photons.

Signal-to-idler energy conversion from 1.9 to 2.3 µm by transient stimulated Raman chirped-pulse amplification

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The combination of optical parametric and transient stimulated Raman amplification of chirped pulses demonstrates a novel approach for idler energy buildup in the mid-IR range. Optical parametric chirped-pulse amplification (OPCPA) output pulses in the wavelength range 1.8–2 µm for the signal and 2.1–2.4 µm for the idler were used as pump and Stokes seed, respectively, in a stimulated Raman amplifier, based on a KGW crystal. Both OPCPA and its supercontinuum seed were pumped with ~1.2-ps pulses from a Yb:YAG chirped-pulse amplifier. The transient-stimulated Raman chirped-pulse amplifier provides a 33% increase in idler energy with nearly transform-limited ~53-fs pulses after compression.

Optimizing self-seeded perfluorooctane SBS-compressor configurations to achieve ~90 ps high-energy pulses

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Three stimulated Brillouin scattering (SBS) configurations in perfluorooctane were experimentally compared to achieve the ultimate compression of ~1.1 ns pulses from a commercial Nd:YAG mini-laser. The 93 ps pulses with an energy of 9.5 mJ were achieved at the output of the double-pass phase-conjugated Nd:YAG amplifier. The resulting diffraction-free, high-quality beams with M^2 ~1.2 and excellent pointing stability are of practical interest for scientific, medical and industrial applications.

Femtosecond laser wavelength-dependent formation of plasmonic gold nanostructures

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Formation of gold nanobumps, nanocones, and nanojets using laser direct writing techniques and varying laser wavelengths was investigated. The wavelength of laser irradiation impacted the size and shape of fabricated structures, as well as the minimum achievable grating period, layer modification fluence, and formation fluence range. It has been observed that reducing the wavelength provides a more accurate fabrication process and

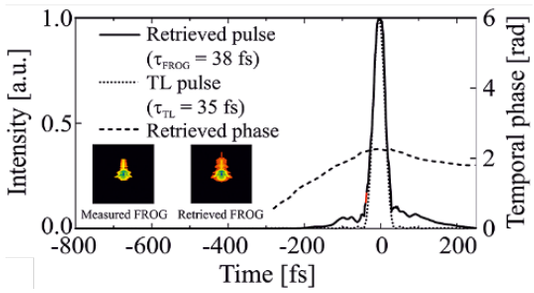

Fig. 1. Temporal profile and phase of the compressed pulse at maximum output energy retrieved by SHG-FROG compared to the transform-limited pulse.

https://doi.org/10.1017/hpl.2023.24

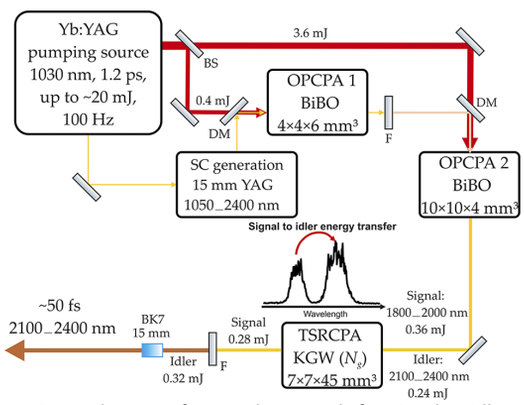

Fig. 2. Experimental setup of a novel approach for signal-to-idler energy conversion.

https://doi.org/10.1364/OL.481811

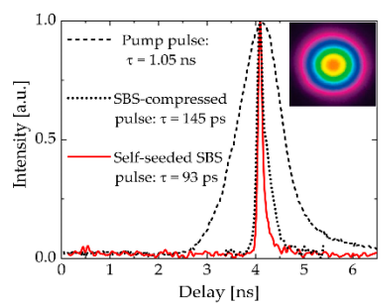

Fig. 3. Temporal shapes of SBS-compressed pulses with a plane feedback mirror, without it, and a pump pulse; (inset) near-field output beam intensity profile.

https://doi.org/10.3390/photonics10091060

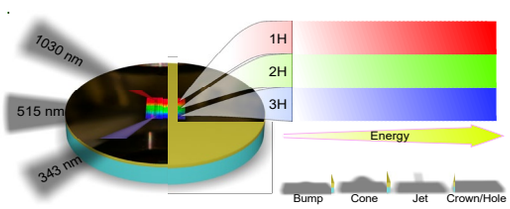

Fig. 4. Graphical abstract of the research.

allows better control of material properties. The gratings of the wavelength-dependent nanostructures induce high quality hybrid lattice plasmon resonances and show great practical potential.

https://doi.org/10.1016/j.apsusc.2023.156629

Single-shot image-fusion upsampling of fluorescence lifetime images

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Fluorescence lifetime imaging is an important tool in bio-imaging that enables to detect subtle changes in cell dynamics and their environment. Most time-domain approaches currently involve scanning a single illumination point across the sample, which can make imaging dynamic scenes challenging, while single-shot "rapid lifetime determination" can suffer from large uncertainties when the lifetime is not appropriately sampled. Here we propose a time-folded fluorescence lifetime imaging microscopy (TFFLIM) approach, whereby a time-folding cavity provides multiple spatially sheared replicas of the lifetime, each shifted temporally with respect to a fixed time-gate. This provides a robust, single-shot FLIM approach that we experimentally validate across a broad lifetime range on fluorescent beads and Convallaria samples.

https://doi.org/10.1073/pnas.2214617120

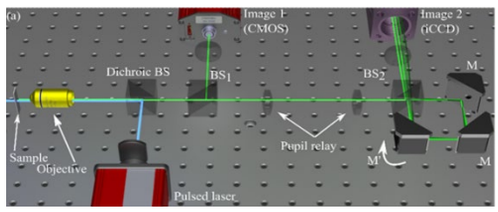

Fig. 5. The system consisting of an objective with epi-fluorescence illumination, two cameras (standard CMOS, and a gated iCCD), and a time-folding optical cavity.

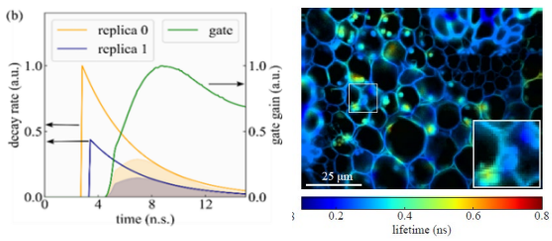

Fig. 6. (Left) Replicas of the signal with an added time lag caused by the round-trip time of the cavity. (Right) The 8x8 upsampling of convallaria image.

Inverse-designed photonic crystals for spatial filtering

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Zero incidence angle spatial filters of a compact design could be useful for intracavity spatial filtering in high-power micro-lasers. Typically, micro-lasers, especially in high-power operation regimes, emit beams of low spatial quality due to the large aspect ratio of the laser resonator. Compact spatial filtering is possible by integration of Photonic Crystal structures into the micro-resonator of the laser. We report efficient spatial filters with desired filtering properties engineered by the inverse design. Such filters could be designed not only separately for both polarizations of the incident radiation, but also simultaneously for both S and P polarizations. The inverse-designed structure was manufactured by physical vapour deposition. It highlights a good correspondence between the angle-wavelength transmission map and the target one.

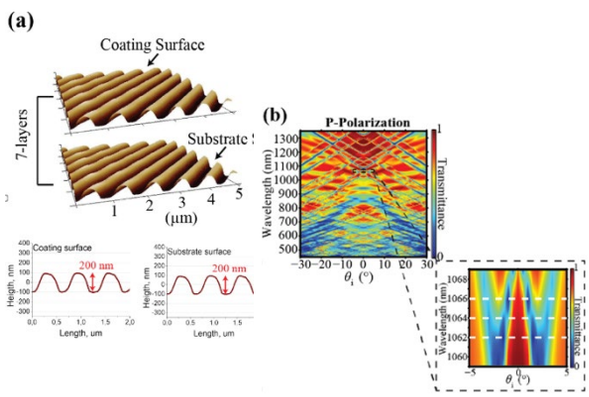

Fig. 7. (a) The surface profile measured by AFM before and after the deposition process. (b) Transmission maps in the angle and wavelength plane.

https://doi.org/10.1063/5.0150756

Extremely narrow sharply peaked resonances at the edge of the continuum

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We report a critical narrowing and sharpening of resonances of a potential well when their eigenfrequencies approach the edge of the continuum. The resonances also obtain sharply peaked shapes with the discontinuity of their slopes. The situation can be realized for an electromagnetic wave propagating across dielectric thin films with a periodically modulated interface(s). We show the phenomenon semi-analytically on a general model of a driven quantum potential well and also by rigorous numerical analysis of Maxwell equations for the wave propagation across the thin film with a modulated interface(s). We corroborate the phenomenon experimentally by measurements of light reflection from a dielectric thin film deposited on a periodically modulated surface.

https://doi.org/10.1103/PhysRevA.107.L061501

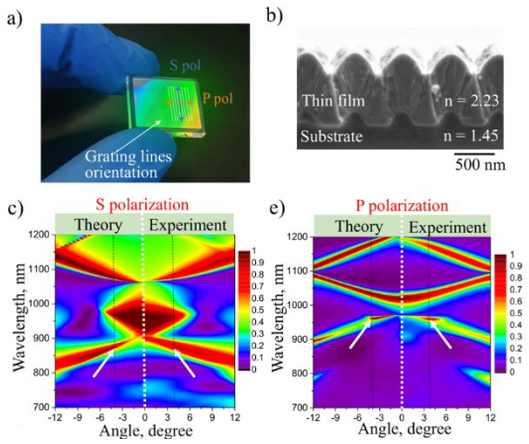

Fig. 8. (a) Fabricated sample, (b) the SEM image of the sample cross-section, (c,d) numerical and experimental maps of the reflection in the plane of angle and wavelength.

Anti-reflective coatings produced via atomic layer deposition for hybrid polymer 3D micro-optics

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The increasing demand for optics quality requires the lowest optical power loss which can occur from unwanted reflections. Laser direct writing (LDW) for the fabrication of complex structures is particularly advantageous in micro-optic applications. This research demonstrates the possibility of forming an anti-reflective coating on hybrid polymer micro-lenses fabricated by employing LDW without changing their geometry. Such coating deposited via atomic layer deposition (ALD) decreased the reflection from 3.3% to 0.1% at a wavelength of 633 nm for one surface of hybrid organic-inorganic SZ2080™ material. This research validates the compatibility of ALD with LDW 3D multiphoton lithography synergistically, expanding its applications on optical grade sub-100 µm scale micro-optics.

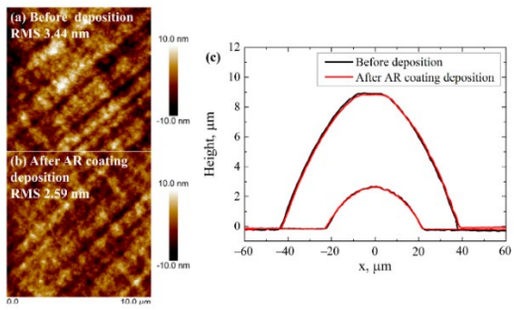

Fig. 9. Surface morphologies of SZ2080™ microstructures measured with AFM (a) before deposition and (b) after deposition of the anti-reflective coating; (c) profiles of the 45 µm and 95 µm diameter micro-lenses before and after the deposition of the anti-reflective coating.

https://www.mdpi.com/2079-4991/13/16/2281

Enhancing laser damage resistance of Co^{2+}:$MgAl_2O_4$ crystal by plasma etching

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Co^{2+}:$MgAl_2O_4$ crystals are successfully used as passive Q-switches within the cavity of erbium glass lasers. Their limited resistance to laser radiation might also put constraints on the generated output peak power. The research demonstrates low-energy plasma etchings of crystal surfaces using different depths of 50, 100, 250 and 400 nm. The laser-induced damage threshold (LIDT) increase of 5-6 times for etchings of 100 nm and deeper was obtained with minimum initial surface roughness deterioration. Effective removal of subsurface damage was also clearly seen using TEM analysis. The results demonstrated a good potential of oxygen plasma etching for obtaining highly laser-damage resistant Co^{2+}:$MgAl_2O_4$ crystals for high-power laser applications.

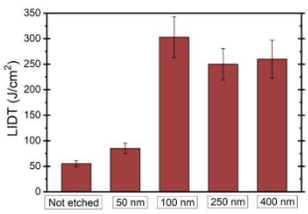

Fig. 10. Surface LIDT (R(1)-on-1) for 1064 nm (τ=3.5 ns, d=55 µm) of unprocessed and plasma-etched to different depths Co^{2+}:$MgAl_2O_4$ crystals.

https://doi.org/10.3390/app13021150

Significant enhancement in laser damage resistance of YAG crystal surface by plasma etching

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The high-quality surface of the optical element is a prerequisite for a high-power laser system design. Yttrium aluminium garnet (YAG) crystal is the critical material for solid-state laser active medium. Laser-induced damage threshold (LIDT) of the YAG crystals might substantially limit the maximum output power of the whole laser system. A novel possibility for significant LIDT enhancement is via plasma etching of YAG crystal surface for picosecond laser pulse durations. The dependence of the LIDT on the etching depth was investigated. With the optimized etching conditions, the LIDT value increased more than 3 times and reached the intrinsic LIDT of the bulk crystal.

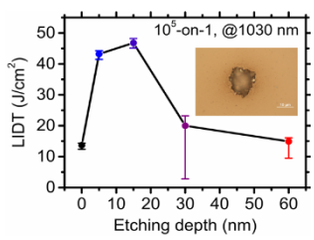

Fig. 11. Summary of LIDT dependency on the etching depth. (Inset) The example of a laser damage morphology for YAG.

https://doi.org/10.1364/OL.484704

Growth of magnetron-sputtered ultrathin chromium films: in situ monitoring and ex situ film properties

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We report a systematic nanoscale investigation of the ultrathin Cr film growth process and film properties. Polycrystalline metallic films were manufactured by magnetron sputtering on fused silica substrates. The film growth was observed in situ by broad-band optical monitoring (BBM) and plasma-emission spectroscopy (OES) methods. The ex-situ characterization of the Cr films, of thickness varying from 2.6 nm up to 57 nm, was performed by both non-destructive and destructive techniques. Recently, we obtained a novel set of data of optical and electrical properties of sputtered chromium films.

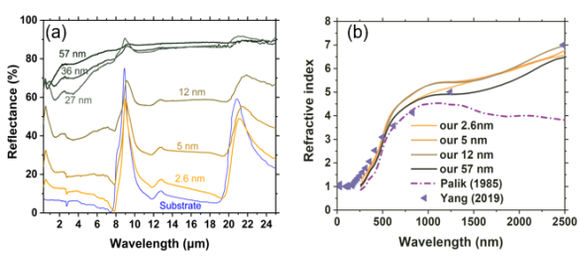

Fig. 12. (a) Reflectance for films with various thicknesses up to far IR range, (b) determined novel optical constants of ultrathin Cr films.

https://doi.org/10.3390/coatings13020347

Optimised spintronic emitters of terahertz radiation for time-domain spectroscopy

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Thin films of spintronic metal excited by femtosecond laser pulses have recently emerged as excellent broadband sources of terahertz (THz) radiation. Unfortunately, these emitters transmit a significant proportion of the incident excitation laser, which causes two issues: first, the transmitted light can interfere with measurements and must be attenuated; second, the transmitted light is effectively wasted as it does not drive further THz generation. Here, we address both issues with the inclusion of a high-reflectivity (HR) coating made from alternating layers of SiO_2 and Ta_2O_5. Emitters with the HR coating transmit less than 0.1% of the incident excitation pulse. Additionally, we find that the HR coating increases the peak THz signal by roughly 35%, whereas alternative attenuating elements reduce the THz signal. To further improve the emission, we study the inclusion of an antireflective (AR) coating to the HR-coated emitters and find the peak THz signal enhanced by 4%.

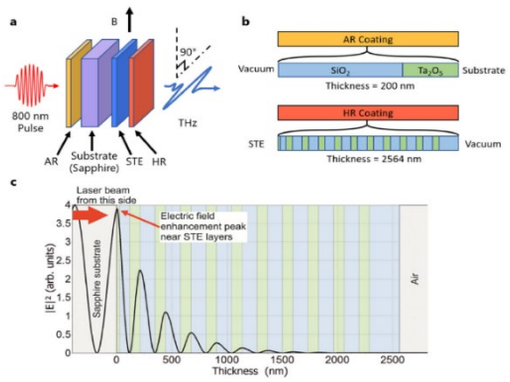

Fig. 13. (a) Schematics of an AR+HR-coated spintronic THz emitter. The emitter is in a magnetic field, B, parallel to the emitter surface. (b) Diagram of the layers in the AR and HR coatings. (c) Electric-field profile of the HR coating.

https://doi.org/10.1007/s10762-022-00897-9

Relativistic laser third-harmonic generation from magnetized plasmas under a tapered magnetostatic wiggler

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Third harmonics generated by Gaussian laser pulse, propagating in magnetized plasma under the impact of tapered magnetostatic wiggler field, is studied. Fundamental equations for analysis of third-harmonic generation are derived, by employing the equation of motion, the continuity equation, and the perturbation technique for Gaussian laser pulse in a weakly relativistic regime and the attendance of a wiggler magnetic field. Additionally, the effects of laser strength, wiggler field, plasma frequency, and the d-parameter on the third-harmonic generation are investigated. The results show that the amount of a wiggler frequency required to generate the third harmonics decreases with an increase in the laser strength parameter. The plasma frequency is enhanced with increasing wiggler frequency. The efficiency of the generated third harmonics decreases with increasing d-parameter. It is found that the efficiency of the generated third harmonics also depends on the time, and the maximum efficiency occurs while the phase matching condition is satisfied. The efficiency of the generated third harmonics is enhanced with increasing plasma frequency. Moreover, it is revealed that the Gaussian laser pulse amplitude has a negligible effect on the third-harmonics efficiency at very low intensities.

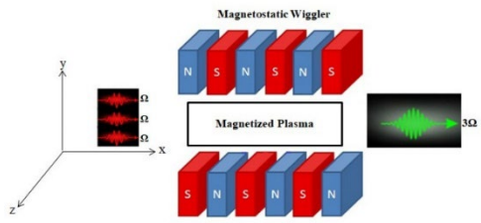

Fig. 14. (a) Schematics of an AR+HR-coated spintronic THz emitter. The emitter is in a magnetic field, B, parallel to the emitter surface. (b) Diagram of the layers in the AR and HR coatings. (c) Electric-field profile of the HR coating.

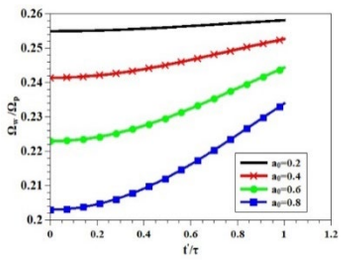

Fig. 15. Variation of the normalized wiggler frequency (Ω_w/Ω_p) with respect to variation of (t'/τ).

https://doi.org/10.1063/5.0155016

Investigation of the modification properties in fused silica by deep-focused femtosecond pulses

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We demonstrate the elongated Type I modifications in fused silica with an axial length > 50 µm. Such extended longitudinal dimensions were obtained by deep focusing radiation of a femtosecond laser inside fused silica at a depth of 2 mm. The transition from the Type II modification (nanogratings) to the Type I modification (refraction index change) was observed with increasing focusing depth at the constant pulse energy. The refractive index changes of ~1.5×10^{-3} for a single pass and 2.4×10^{-3} for multiple passes were demonstrated. The radial dimensions of the deep-focused modifications were confined to 0.5-1.5 µm. By overlapping the modifications in radial and axial directions, the 1D phase grating in the depth range from 2 to 5 mm was recorded, allowing to split the beam with a diffraction efficiency of > 96%. We demonstrate that the aberration-based recording with a Gaussian beam in fused silica is a simple tool for fabricating complex phase diffractive optical elements.

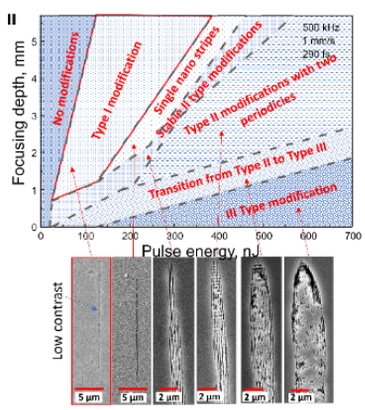

Fig. 16. Modification morphologies for various focusing depths and pulse energies: the classification map of the modifications recorded with 1 mm/s scan speed, 500 kHz repetition rate and 290 fs pulse duration.

https://doi.org/10.1364/OE.477343

Fabrication of a multilevel Fresnel axicon deep in fused silica by femtosecond laser machining

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A simple approach to the manufacturing and optimization of a multilevel phase-only diffractive conical lens (Fresnel axicon or “fraxicon”) was demonstrated. The method for recording deep Type I modifications in fused silica was established and its ability was proven. We showed the prospects and limitations of elements processed using this method. The fine and advanced parameters optimization allowed us to get a compensation mechanism for almost uniform change of refractive index for each separate layer. The maximum diffraction efficiency of the fraxicon for a wavelength of 515 nm was ~80%. The measured Bessel beam depth of field was compared with commercially available conical lens axicons and demonstrated good agreement.

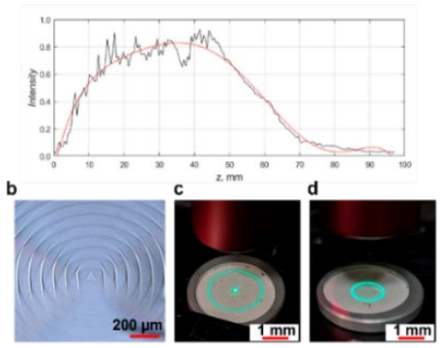

Fig. 17. (a) The quasi-Bessel beam intensity distribution along the beam propagation direction and its intensity cross sections. (b) The microscope picture of recorded fraxicon in the volume of fused silica. (c) Far-field picture of Bessel beam from fraxicon and (d) refractive axicon after microscope objective.

https://doi.org/10.1364/OL.498853

Etching peculiarities in sapphire induced by double-pulse irradiation with variable delay and crossed polarisation

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The results of the intra-volume modifications and etching peculiarities of bulk crystalline sapphire (α-Al_2O_3), induced by double-pulse femtosecond laser radiation with a variable delay between pulses, were presented. The selective etching of sapphire was tested using various combinations of double-pulse irradiation. It was demonstrated that by varying the inter-pulse delay from -10 ps to 10 ps, the enhanced etching rate of the sapphire microchannels could be achieved compared to the single-pulse processing. It was demonstrated an asymmetrical etching behaviour versus inter-pulse delay, depending on polarisation of the first pulse relative to the scan direction (positive and negative pulse delays), when etching proceeds only in hydrofluoric acid (HF). In order to etch the entire structure, a combination of HF and a solution of H_3PO_4: H_2SO_4 (3:1) was used. The isotropic etching

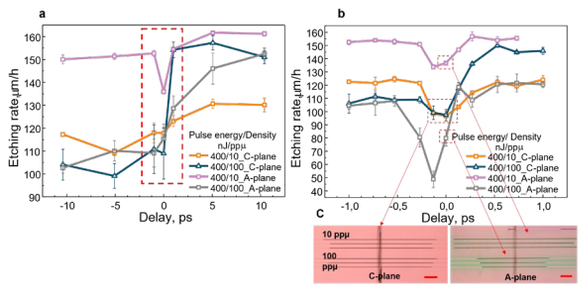

Fig. 18. (a) Etching rate dependence in the C-plane and A-plane sapphire samples on the inter-pulse delay ranging from -10 ps to 10 ps. (b) A detailed etching rate investigation in the range from -1 ps to 1 ps marked by the red square in Fig. 18a. (c) The microscope pictures of the etched microchannels 150 µm below the sample surface for 0 ps inter-pulse delay for the C-plane and A-plane sapphire. The first (second) number in the insert shows pulse energy (pulse density). The red scale bar represents a distance of 100 µm.

properties of H_3PO_4: H_2SO_4 made it possible to release items from the crystalline portion of the sapphire.

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Polarization-dependent four-port fibre optical circulator based on the Sagnac effect

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A fibre optic circulator with a rotating ring interferometer based on the Sagnac effect was proposed and investigated. A ratio of 104:1 in light transmittance in the forward and backward directions between the same input/output ports of the circulator was experimentally demonstrated. The optical isolation in the backward direction was 24 dB. The Sagnac circulator in the free-space configuration could be adapted for particularly high optical powers because it does not contain optical components

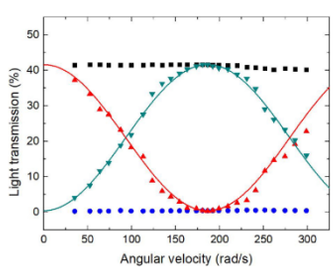

Fig. 19. Light transmittance between different circulator ports depending on the rotational velocity of the ring interferometer.

susceptible to thermal effects or optical damage, in contrast to conventionally used devices based on magneto-optical materials.

https://doi.org/10.1364/OE.476262

Regenerative shaper of ultrashort light pulses

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An ultrashort light pulse regenerative shaper based on a closed-loop double-stage Mamyshev regenerator with an electrically controllable acousto-optic switch was proposed and investigated. This type of setup allows to apply an initial pulse from an external pulse source and reshape the pulse to an ultrashort high-quality compressible one due to repeated pulse round-trips in the closed-loop regenerative circuit.

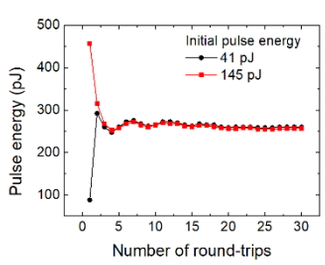

Fig. 20. The energy of the regenerated pulse versus the number of round trips.

https://doi.org/10.3390/photonics10070836

Generation of gold and silver nanoparticles using laser ablation of thin bimetallic films and bulk targets in water

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We demonstrated the generation of hybrid gold-silver nanoparticles using the laser ablation of thin-film composites on a glass substrate in water and compared with the laser fabrication of nanoparticles by using bulk targets of silver and gold. Thin-film method allows the formation of stable hybrid Au–Ag nanoparticles in distilled water without any stabilizers and additional ligands with an opportunity to regulate the nanoparticle composition using different metal ratios, layer order, and thickness of films. The stability and optical properties of the hybrid nanoparticles depend on the laser pulse energy used. This study demonstrates that the thin film method produces nanoparticles with higher stability compared to the bulk target method.

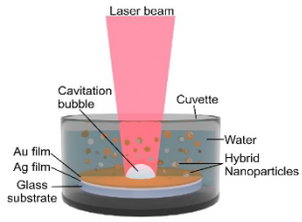

Fig. 21. Gold-silver nanoparticle generation using laser ablation in water.

https://doi.org/10.1016/j.optmat.2023.113535

Efficient surface polishing using burst and biburst mode ultrafast laser irradiation

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The use of laser irradiation for micromachining is widely applicable and has many benefits. One of the main uses is that it is possible to mill and polish the sample using the same laser system. State-of-the-art laser systems with high average optical power and burst regimes are widely applied in technology. The main advantages of burst regimes are the fluence values closer to optimal ones and residual heat reusage for subsequent pulses. In this study, the influence of MHz burst, GHz burst, and bi-bursts was investigated for significant surface polishing of copper and stainless-steel samples. The Z-scan experiments were performed to determine the optimal number of sub-pulses inside the burst for the lowest surface roughness.

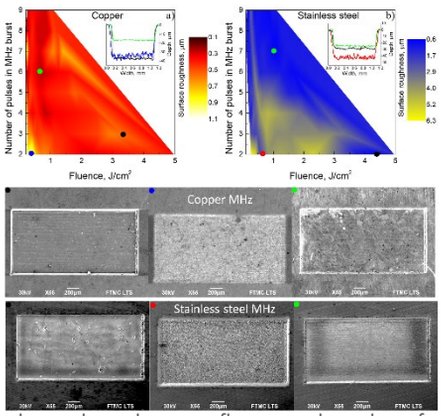

Fig. 22. Surface roughness dependence on fluence and number of pulses in the MHz burst for (a) copper and (b) stainless steel. Scanning electron microscope pictures are shown for indicated colour dots.

https://doi.org/10.1039/D2RA05208C

Laser-induced graphene in polyimide for antenna applications

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Laser-induced graphene (LIG) has gained considerable attention recently due to its unique properties and potential applications. The LIG-PI composite material was prepared by a picosecond laser (1064 nm) irradiation process, which resulted in a conductive graphene network within the PI matrix. LIG formation was confirmed by Raman spectroscopy and sheet resistance measurements. Finally, a patch antenna from LIG with 2.45 GHz microwaves was simulated, produced, and tested. These findings suggest that LIG-PI can provide a new avenue for developing flexible and wearable high-frequency electronics.

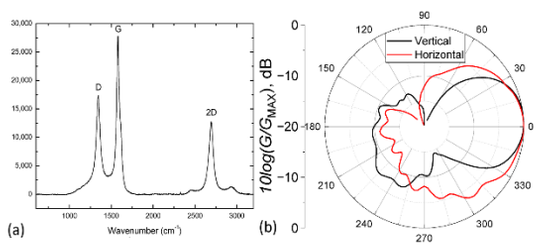

Fig. 23. (a) Raman spectrum of LIG, formed using a 148 J/cm^2-irradiation dose and possessing the lowest sheet resistance of 36.6 Ω/sq. (b) The directivity of antenna.

https://doi.org/10.3390/cryst13071003

GaAs ablation with ultrashort laser pulses in ambient air and water environments

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In this study, we investigated femtosecond laser ablation of deep trenches in GaAs, an important optoelectronic material, using water and ambient air environments at different laser processing regimes. We applied surface morphological analysis, atomic-resolution transmission electron microscopy imaging, elemental mapping, photoluminescence, and Raman spectroscopy. Findings demonstrate that the GaAs ablation efficiency is enhanced in water as well as processing quality. Furthermore, Raman spectroscopy revealed a reduced presence of amorphous structure within the ablated trenches.

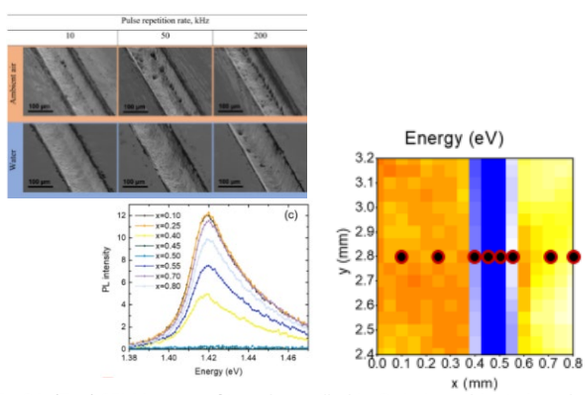

Fig. 24. (Top) SEM images of trenches milled in GaAs in ambient air and water at different processing regimes. (Bottom) Room-temperature PL spectra at eight different positions taken from the trench ablated in water at 10 kHz.

https://doi.org/10.1063/5.0152173

Femtosecond laser cutting of borosilicate glass in ambient air and water

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The cutting quality and strength of strips cut with pulses of 350 fs duration were investigated for different thicknesses (110 - 550 µm) of borosilicate glass plates. Cutting was performed in two environments: ambient air and water. Laser cutting parameters were individually optimized for different glass thicknesses and cutting environments. The results revealed that cutting in water was favourable for thicker glasses (>300 µm) yielding higher cutting quality, higher effective cutting speed and characteristic strength. The cutting of ultrathin glasses (110 µm) demonstrated almost identical performance and cutting quality in both environments.

https://doi.org/10.3390/mi14010176

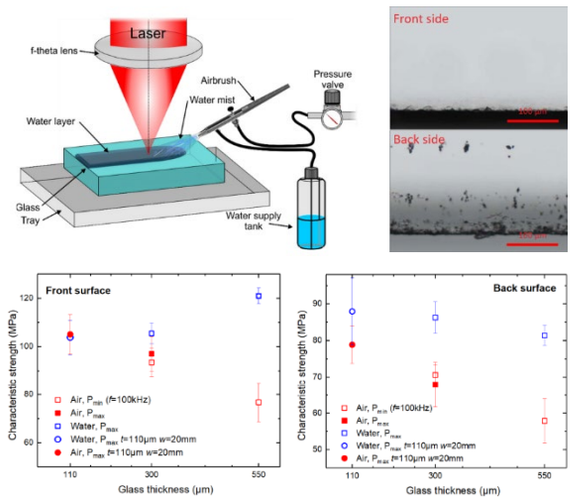

Fig. 25. (Top, left) Setup for glass cutting in water. (Top, right) Typical front and back side edge quality of glass strips cut in water. (Bottom) Characteristic strength of laser-cut glass strips. Bending force applied from the front (left) and back (right).

Laser wakefield acceleration of electrons using Bessel–Gauss doughnut beams for accelerating beam guiding

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Plasma density structures, created by high-order Bessel–Gauss beams for guiding the accelerating Gaussian beam and laser wakefield acceleration of electrons, are analysed using Wake-T and Fourier–Bessel particle-in-cell (FBPIC) simulation tools. The Gaussian beam at the acceleration distance of 2 mm in the plasma concentration of $n_0 = 3 \times 10^{18}$ cm^{-3} diffracts substantially, and the waist radius of the laser beam increases. The guiding of the Gaussian beam with a_0 =5.0 by the B_2G beam with a_0 =1.5 increases the propagation distance. The average energy of electrons is by a factor of 2.3 higher, and the divergence is 1.7 times lower compared to the Gaussian beam parameters. The maximum electron energy reaches 283±83 MeV at the acceleration distance of 2 mm.

https://doi.org/10.1017/S0022377823000247

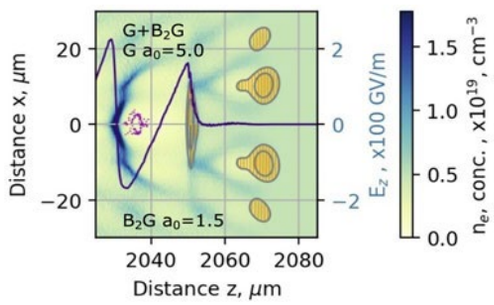

Fig. 26. (Colour map) Distribution of plasma concentration and (line) dependence of longitudinal plasma wake electric field Ez formed behind the Gaussian beam with a_0 =5.0 guided by the B2G beam with a_0 =1.5. Isolines with yellow oscillating lines represent the location and intensity of the electrical field of the laser pulses. The violet cloud is the electron bunch injected behind the laser pulse.

Carrier-envelope phase-controlled dynamics of relativistic electron beams in a laser-wakefield accelerator

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In laser wakefield acceleration, an ultra-intense laser pulse is focused into an underdense plasma to accelerate electrons to relativistic velocities. For single-cycle pulses, the ponderomotive approximation of the laser envelope breaks down, and the actual waveform of the laser has to be taken into account. The laser-plasma acceleration (LPA) is significantly impacted by the laser carrier-envelope phase and, to achieve stable acceleration in both pointing and beam charge, the carrier envelope phase (CEP) stabilization is required. In both nitrogen and helium plasma, we observed variations of the electron beam pointing by order of 10 mrad in the polarization direction as well as 30% variations of the beam charge locked to the controlled laser CEP. Our simulations indicate that the periodically injected bunches are particularly short, have low emittance and are particularly interesting for ultrashort X-ray betatron radiation sources due to their off-axis injection.

https://doi.org/10.1140/epjs/s11734-022-00675-7

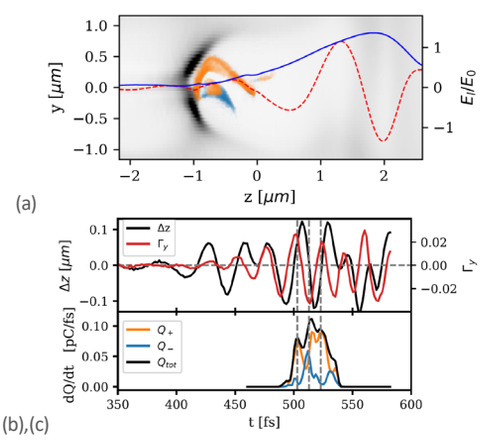
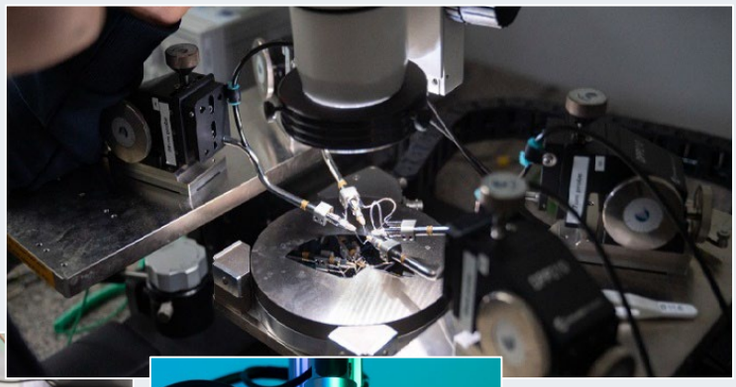
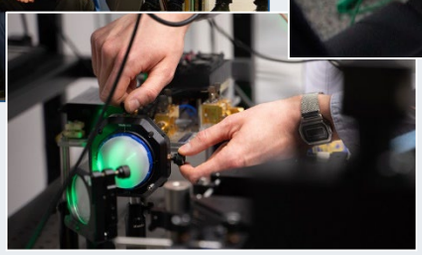


Fig. 27. Particle-in-cell simulation of an LPA driven by a 4.0 fs laser in a helium plasma. (Top) Snapshot of the wakefield for an initial CEP of 0, showing three different injected sub-bunches. Electron density is shown in grey, and injected electrons are displayed in orange and blue. The normalized laser electric field is shown by the red and its envelope - by the blue line. (Bottom, up) Time dependences of the wakefield in the y-direction (red line) and the difference in the mean position of the bubble Δz (black line). (Bottom, down) Charge injection rate. The grey dashed lines highlight the three main injection events.





Department of Optoelectronics

Prof., Habil. Dr. Gintaras Valušis
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The scientific and technological activities of the Department in 2023 were balanced between the fundamental and applied research. The main scientific directions were terahertz (THz) technologies and semiconductor nanomaterials engineering. The studies in first direction were focused mainly on the development in imaging and spectroscopic systems with the aim to reduce their size; in particular, on search of diffractive optics solutions and studies of semiconductor quantum superlattices as a gain media for high-frequencies room temperature operation. The second direction relies on materials engineering of A3B5 nanostructures grown by molecular beam epitaxy (MBE) employing two apparatus by SVT and Veeco available at the Department. The fabricated nanostructures, such as GaAs/AlGasBi and GaInAsBi nanocompounds, are studied optically, and then, after relevant processing, can be further used for various applications, for instance, for the development of infrared LEDs and lasers as well as novel semiconductor nanostructure based solar cells. The previous year studies of 2D materials were successfully continued – several-atom-thick layers of Bi, bismuthene, and its properties gained our additional attention. It is noteworthy several new activities which started this year. Our efforts were focused on optimization process of multiple InGaAs quantum wells grown for vertical-external cavity surface emitting laser (VECSEL) applications. A significant correlation was revealed between emitted light intensity and wavelength, offering a detailed study of the effect of structural dislocations on optical quality. Employing both laser confocal microscopy and spectrometry, the chart of microphotoluminescence (μPL) intensity variations, associated with the emission wavelength across the sample due to the presence of dislocations, was obtained. These observations are of particular importance for semiconductor manufacturing, where the control of dislocation densities is crucial in optimizing the performance of photonic devices, such as high power VECSELs. Also, special attention was paid on the investigation of nonparaxial silicon-based diffractive optics components for the development of compact THz imaging systems aiming to find rational design for assembling optical setups. These studies were performed in a close cooperation with the Department of Fundamental Research. Finally, Dr. Tadas Paulauskas, a member of our Department, was one of the key-drivers initiating quantum technologies related activities in Lithuania. The Departmental structure experienced some changes during last year: to concentrate our activities, the Laboratories of Ultrafast Optoelectronics and Optoelectronics Technology were merged, and a new Laboratory of Photonic Technologies and Devices was established. It became a new constituent of the Department along with Laboratories of Semiconductor Optics, Terahertz Photonics, and Optoelectronic Systems Characterization.

Last but not least, Professor, Academician of the Lithuanian Academy of Sciences, Habil. Dr. Arūnas Krotkus retired from the Department this year. He was one of the scientific leaders of our Department, the pioneer of ultrafast studies in semiconductors and the initiator of semiconductor materials engineering and bismuth compounds technology in Lithuania. Currently, he holds a position of FTMC emeritus scientist and still shares his experience, scientific knowledge and erudition with younger collegues discussing new activities and projects. We highly appreciate his versatile support.

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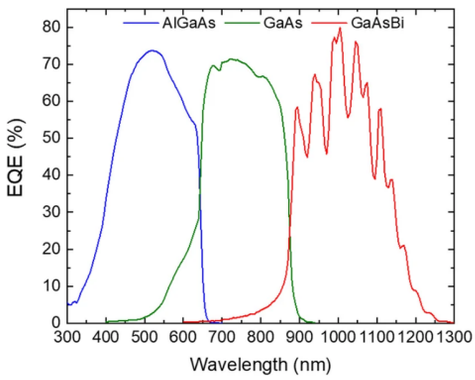
Performance assessment of a triple-junction solar cell with 1.0 eV GaAsBi absorber

Multijunction solar cells, utilizing group III-V semiconductors, are extensively employed in space applications due to their high efficiency and radiation resistance. To enhance their properties further, integration of new materials with more optimized energy bandgaps is being pursued. The Department of Optoelectronics has produced the world's first multijunction thin-film AlGaAs/GaAs/GaAsBi solar cell, featuring an optimal 1.0 eV energy bandgap GaAsBi bottom junction. Moreover, this solar cell exhibits a simpler architecture, owing to the lower lattice mismatch of the GaAsBi crystal with the top junctions. These advancements pave the way for the development of bismide-based multijunction solar cells with efficiencies well above 30%.



External quantum efficiency (EQE) plot of a triple-junction AlGaAs/GaAs/GaAsBi solar cell.

https://doi.org/10.1186/s11671-023-03865-x

Electro-Optical THz beam modulator based on drifting space-charge domains in GaN semiconductors

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Electro-optical modulation of THz beam was found in n-type GaN epilayers under pulsed electric field excitation. Proposed Electro-Optical THz modulator is composed of a 10 μm thick lightly doped GaN epilayer grown on a c-plane of a native semi-insulating substrate. Two contacts are used to drive the n-GaN epilayer into a regime of drifting space-charge domains, and their high internal electric field (peak values reach above 200 kV/cm) efficiently modulates transmission through the GaN semiconductor. The modulator is sensitive to beam polarization demonstrating a nonlinear increase of THz transmission up to 50 % under the external electric field value up to 1.6 kV/cm, only. Rough estimates indicate that maximum values of operational frequency and power density for such component could reach up to 60 MHz and 1 W/cm2, respectively. This is a joint research with UNIPRESS, Warsaw, Poland.

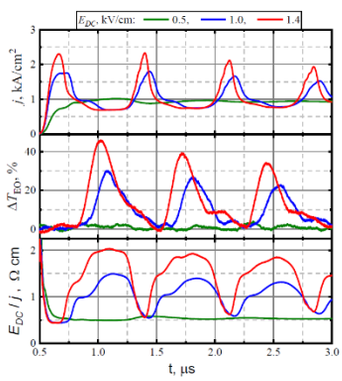

Fig. 1. Traces of charge current density j, the electro-optic modulation of 0.6 THz frequency beam transmission ΔT_{EO}, and the sample specific resistance, E_{DC}/j.

https://doi.org/10.1063/5.0152661

Directive and coherent thermal emission of hybrid surface plasmon-phonon polaritons (SPPhPs) in GaN

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Beaming and coherent thermal emission of SPPhPs was numerically and experimentally observed in the n-GaN surface relief gratings (SRGs) shaped in a linear and radial geometry. Polariton propagation losses were minimized and the spatial and temporal quality of the selected mode radiation in a normal direction was maximized by fixing the grating period value at 17.5 μm and varying the grating filling factor from 75% to 25%. A set of optimal design linear and radial geometry SRG samples were fabricated validating modelled emission characteristics of hybrid SPPhPs. For the first time we demonstrated, without the use of extra focusing optics, that both the efficient emission and the beaming can be achieved due to excitation and interference of the same number but opposite sign polariton modes in n-GaN SRG.

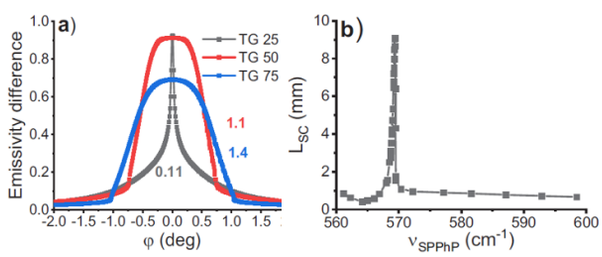

Fig. 2. (a) Directivity characteristic of n-GaN gratings with various filling factors at their peak emission frequency towards normal direction. Numbers near each curve show FWHM values in cm^{-1} units. (b) Coherence length spectrum of the SPPhP emission from TG 25 grating.

https://doi.org/10.1364/OME.494777

Multi-phase Fresnel lenses on semiconductor wafers for THz frequencies

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The multi-phase Fresnel hybrid lenses (H-MPFLs) were developed on silicon wafer at the frequency of 585 GHz. The design of a standard MPFL was modified thoroughly in various outer zone areas in order to reduce complexity and manufacturing time of the diffractive optical elements by employing the direct laser ablation. The phase offset was found by a precise control over the phase shift of incoming radiation in steps of $\pi/12$, revealing its optimal value at $+\pi/4$ independently of the hybridization order of the lens. The focusing gain of hybrid lenses was found to be up to 10 % higher than that achieved with a standard design MPFL. The modelling data were confirmed by experiments demonstrating effective THz beam focusing with H-MPFL samples to the diffraction limited spot size. Proposed approach can be further modified by scaling the hybrid lens design to other frequencies with different zone numbers and/or by using other materials suitable for THz photonics integration on a semiconductor chip.

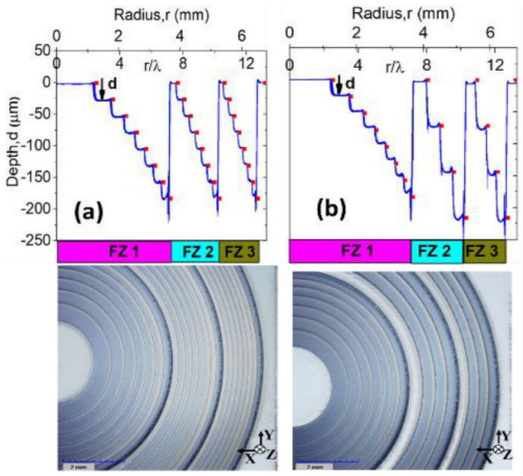

Fig. 3. The step profile across centrum line (top row) and microscope picture (bottom row) of the fabricated MPFL samples of (a) standard design with the phase quantization levels Q=8 for all Fresnel sub-zones; (b) optimized hybrid design with Q = 4 at both FZ2 and FZ3 areas.

https://doi.org/10.1109/TTHZ.2023.3263638

Narrowband thermal terahertz emission from homoepitaxial GaAs structures coupled with Ti/Au metasurface

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We have demonstrated thermal THz emission from GaAs structures coupled with Ti/Au metasurfaces. The *n*-GaAs/GaAs structures were grown by molecular beam epitaxy and top metallic square array was formed using UV laser lithography. The reflectivity and emissivity exhibited resonant behaviour due to magneto-polariton (MP) excitations in the range from 0.7 THz to 1.3 THz, depending on the size of the squares at 25 °C and 390°C, respectively. An equivalent *LC* circuit model was used to describe the spectral positions of MP resonances analytically. Good agreement between the results of simulation and the reflection and thermal emission experiments was achieved. The MP resonance quality factors (Q = 3.3 to 5.2) obtained at room and elevated temperatures are very similar to those inherent to metal-insulator-metal structures and 2D plasmon resonance features at cryogenic temperatures.

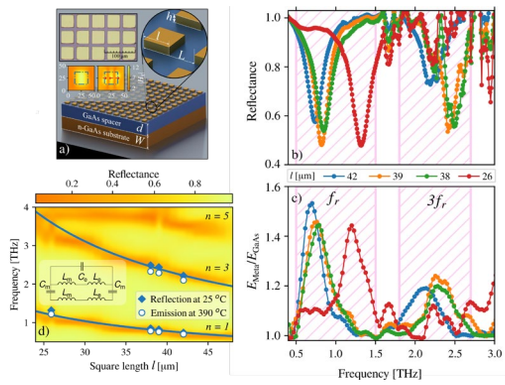

Fig. 4. Panel (a) Structure of thermal emitter. Inset: the photo of metasurface and magnetic field distributions under the square element for the 1st and 3rd resonances. (b) Reflection spectra and (c) thermal emission spectra normalized to the thermal emission of GaAs surface spectra for different square sizes. (d) Dependences of resonant frequency on square size: simulated (colormap), measured (symbols) and calculated (solid curves). Inset: *LC* circuit for resonant frequency calculations.

https://doi.org/10.3390/s23104600

Terahertz radiation helps to reveal semiconductor band structures

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When semiconductor surface is illuminated with femtosecond optical pulses, it emits THz transients with amplitude which allows to determine the energy band structure of the material in considerable detail. To achieve this, the measurements using an optical parametric amplifier as a variable wavelength light source are especially helpful. In this review, the studies of material parameters, such as the energy position of conduction band minima, the energy band offsets in heterojunctions, and the quantum efficiency spectra of multicell solar modules are described.

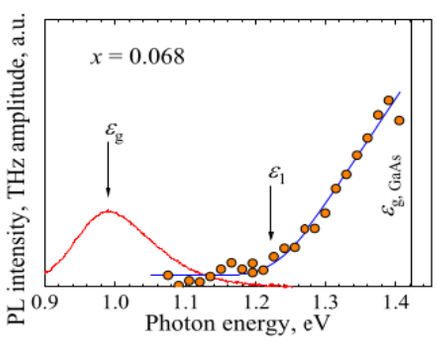

Fig. 5. The THz excitation spectrum in $GaAs_{1-x}Bi_x/GaAs$ heterojunction (orange dots - experiment, blue line - theory). Red line shows the photoluminescence spectrum. Both the energy gap ε_g of GaAsBi and the conduction band offset ε_1 can be determined from these measurements.

https://doi.org/10.3390/ma16072859

Intervalley energy separation in the conduction band of $InAs_{1-x}Bi_x$ determined by terahertz emission spectroscopy

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Terahertz emission spectroscopy was employed to analyze the properties of InAsBi layers in a study of the intervalley energy separation in the conduction band of $InAs_{1-x}Bi_x$. These layers, grown on InAs substrates using molecular beam epitaxy, showed a gradual decrease in the intervalley energy separation as bismuth content increased, with a significant shift noted down to approximately 0.9 eV.

https://doi.org/10.35848/1347-4065/acc777

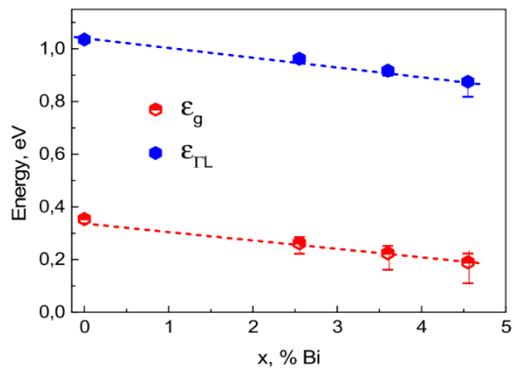

Fig. 6. Experimental values of the energy bandgap and the intervalley energy separation in the conduction band of InAsBi for different Bi content.

Gain mechanisms of high-frequencies in doped semiconductor superlattices

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One of the most challenging issues in implementation of THz frequencies is a lack of powerful and compact emission sources. Semiconductor quantum superlattices due to Esaki-Tsu nonlinearity can be considered a promising option as effective amplifiers of broadband GHz-THz radiation. We explored the case of a high-frequency signal gain, when a probe microwave signal is comparable to the AC pump electric field in a semiconductor superlattice. We identified conditions under which a doped superlattice biased by both DC and AC fields can generate or amplify high-frequency radiation composed of harmonics, half-harmonics, and fractional harmonics. It is demonstrated that in general case the amplification mechanism in superlattices is determined by the coexistence of the phase-independent Bloch and the phase-dependent parametric gain mechanisms. The study showed that the process can be managed by a proper selection of AC and DC electric fields as indicated in Fig. 7 (left). Contribution of these gain mechanisms can be adjusted by sweeping AC pump strength and leveraging a proper phase between the pump and strong probe electric fields. This important finding opens a promising route for novel miniature GHz–THz frequency generators and amplifiers operating at room temperature.

https://doi.org/10.3390/nano13131993

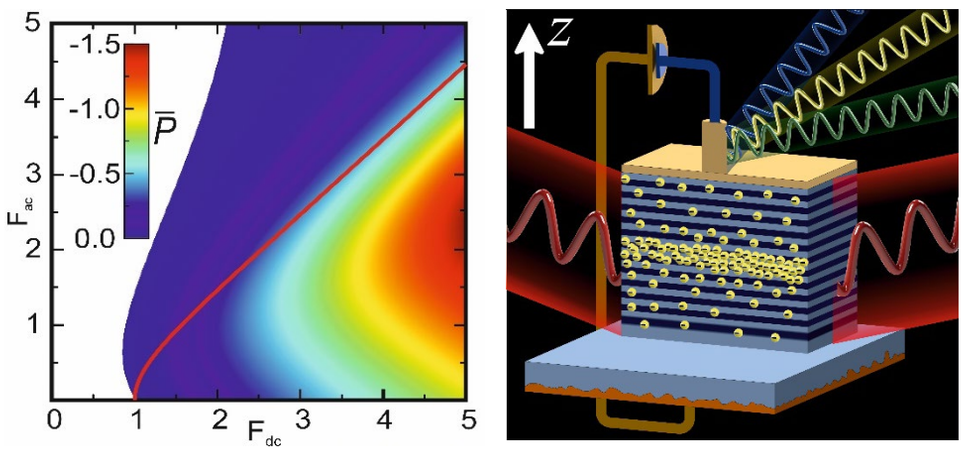

Fig. 7. (Left) Relative power map revealing areas of high-frequency gain for the case of half-harmonics. Red line marks the boundary between the dominating Bloch and the parametric generation processes. (Right) Schematic illustration of the high-frequency gain in a biased semiconductor superlattice.

Department of Molecular Compounds Physics

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The Department of Molecular Compounds Physics is mainly involved in molecular spectroscopy and photonics. Our activities range from the study of natural and artificial molecular systems to the development of molecular and hybrid devices and their characterization techniques. The major objects of our investigations are biological photosynthetic and protein-DNA complexes, molecular aggregates, organic and perovskite solar cells, perovskite light-emitting diodes, perovskite-based light frequency down-converters, other photonic materials and nanostructures important for optical and medical applications. We focus on optically initiated dynamical processes. Therefore, our main tools are time-resolved spectroscopic techniques for studies of ultrafast transient absorption and fluorescence. We combine them with the steady-state optical characterization, optical microscopy, nonlinear microscopy and photoelectric investigations. We strive for a better knowledge of electronic processes in photoexcited materials, nanostructures, interfaces, etc. This is important as for understanding of chemical processes in artificial and natural materials as well as for fabrication of advanced photoelectric devices. We are interested in the evolution of excited states, their properties in excitonically coupled systems, the photogeneration of charge carriers, their motion, trapping, recombination and related processes.

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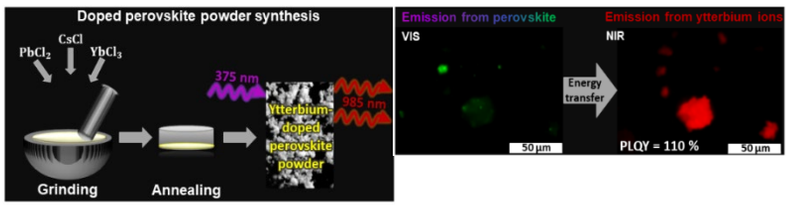
Facile synthesis of ytterbium doped cesium lead halide perovskite powder

Ytterbium-doped perovskites may act as quantum-cutting materials promising in enhancing solar cell efficiency and various other optoelectronic applications. Cesium lead halide perovskites (CLHPs) absorb high energy photons, and their energy can be transferred to ytterbium ions emitting two photons of approximately twice lower energy. Typically, CLHPs are used in the form of nanoparticles or thin spin coated films. We developed a mechanosynthesis technique for easy fabrication of quantum-cutting materials in large amounts. We demonstrate



Left: mechanosynthesis technique for fabrication of ytterbium-doped cesium lead halide perovskite powder. **Right**: fluorescence microscopy images in VIS and NIR regions of ytterbium-doped perovskite powder excited at 405 nm.

https://doi.org/10.1039/D3TC02631K

the formation of ytterbium-doped CLHP powders by dry and wet techniques and examined their structural and optical properties. Both techniques allow doping of the perovskites with ytterbium ions by substituting a fraction of lead ions. The ytterbium doped into the perovskite effectively quenches the excitonic emission and leads to ytterbium photoluminescence efficiencies reaching 160 %.

Electric field-induced quenching of $MAPbI_3$ photoluminescence in PeLED architecture

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We applied electric field-induced photoluminescence quenching to address electronic processes in methylammonium lead iodide perovskite. We distinguished two quenching mechanisms: indirect quenching by field-induced chemical and structural material modifications and direct quenching by the influence of the electric field on the carrier radiative recombination rates. The direct quenching leads to an instantaneous reduction in the radiative carrier recombination rate, by the electron and hole displacement within individual perovskite grains, and spatial separation of electron and hole "clouds" within the entire perovskite layer thickness.

https://doi.org/10.1021/acsami.3c05880

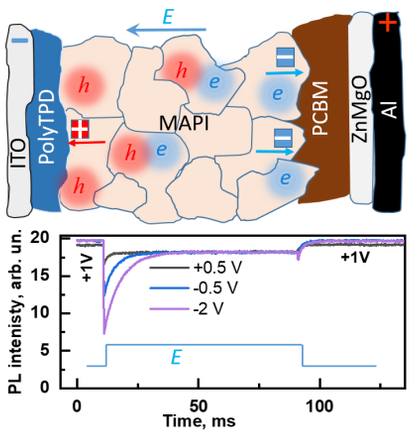

Fig. 1. (Top) Structure of the investigated perovskite PeLEDs. Red and blue squires show accumulation of positive and negative ions, while h and e indicate electrons and holes. (Bottom) The photoluminescence dynamics after application of the voltage pulse.

Stable and reusable lace-like black silicon nanostructures coated with nanometer-thick gold films for SERS-based sensing

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Surface-enhanced Raman scattering spectroscopy (SERS) is one of the most efficient analytical techniques in organic chemistry and biochemistry. However, it suffers from limitations associated with SERS-active substrates, such as their high cost, inherent inhomogeneity and poor long-term stability. We propose a simple, rapid and low-cost method for the preparation of Au-coated black silicon SERS-active substrates with an enhancement factor of 106 and a storage stability of 20 months. The developed SERS-active substrates can be purified and reused at least ten times. This makes them promising tools for laboratory routine research.

https://doi.org/10.1021/acsanm.3c00281

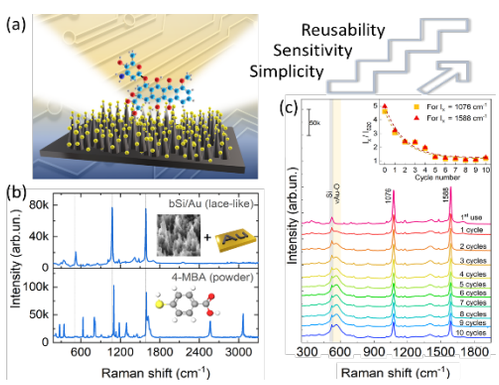

Fig. 2. Application of Au-coated black silicon as a SERS-active substrate: (a) schematic representation, (b) comparison of Raman and SERS spectra of 4-MBA, (c) change in SERS spectra over 10 cycles of substrate use.

Application of artificial neural networks for modeling of electronic excitation dynamics in 2D lattice

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We have analyzed the applicability of deep, sequential, and fully connected neural networks (NNs) to predict the excitation decay kinetics of a simple 2D lattice model, which can represent numerous real-life systems, such as aggregates of photosynthetic molecular complexes. After choosing a suitable loss function for NN training, we have achieved excellent accuracy for predictions of the lattice excitation decay kinetics from the model parameter values.

https://doi.org/10.1063/5.0133711

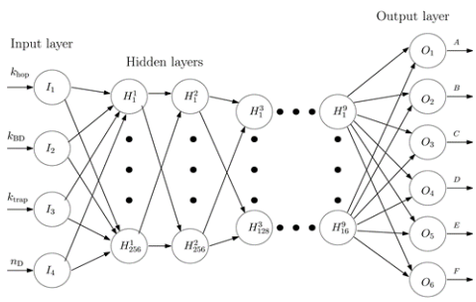
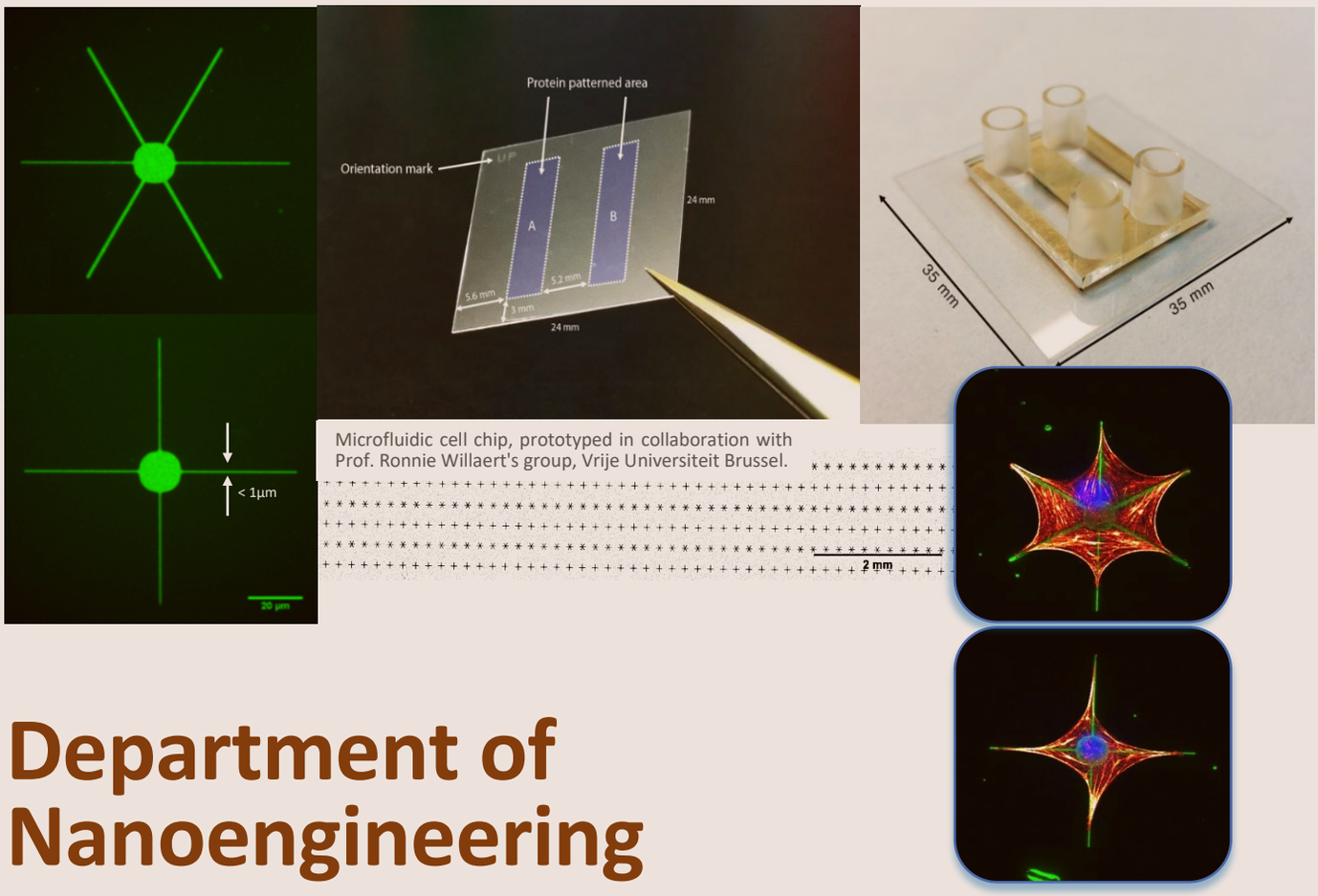


Fig. 3. NN architecture used to predict the excitation dynamics of a 2D system. The lattice parameters (left) are used as the input. The output parameters (right) are the coefficients of the fitting function, which in this case was a sum of two stretched exponentials.



Microfluidic cell chip, prototyped in collaboration with Prof. Ronnie Willaert's group, Vrije Universiteit Brussel.

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 group is successful in international and business collaboration. The competence of the team spans the fields of surface chemistry, materials science, 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 explored in the Department 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 as well as biological and hybrid nanostructures.
- Synthesis of (bi)functional compounds, bioconjugates, and self-assembling blocks.
- Electrochemical sensing of broad range of analytes.
- Carbon nanomaterials, nanoparticle and micro-fabricated electrodes.
- Development and characterisation of conducting polymer materials based on natural monomers.
- 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.

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Efficient direct-write process for surface micropatterning

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We have developed a new approach for creating large-area, microscale resolution surface patterns of specific chemical reactivity (Fig. 1, top). The main idea is based on the local activation of photoacid dispersed in a flat elastomeric stamp by a focused blue laser beam. This allows for generation of acidic "hot spots", thus inducing localized acid-catalyzed chemical reactions on the surface contacting the stamp, while avoiding potentially cytotoxic photochemical reaction products. In contrast to the majority of photolithographic techniques, the method invented herein requires no mask. The resolution of 10 µm can be achieved (Fig. 1, bottom). The use of a visible-light source, as implemented in the commercial inexpensive HD-DVD/Blu-ray hardware as a writing tool, is yet another hallmark of our method. The developed approach has significant potential for biocompatible, cost-efficient surface chemical patterning and biochip technologies.

https://doi.org/10.1021/acsami.2c20568

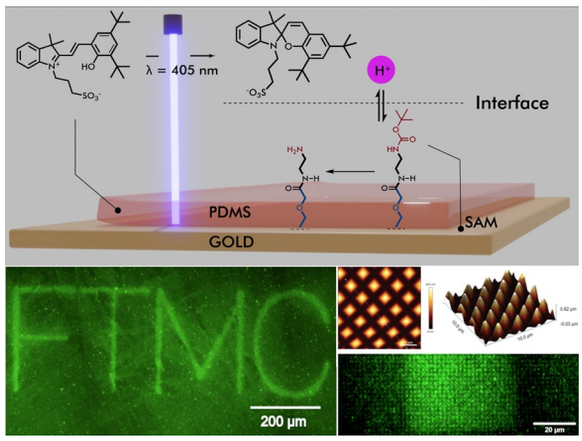

Fig. 1. (Top) Schematic representation of the patterning approach. (Bottom, left) Fluorescence image of the reactive amine pattern. (Bottom, right) Atomic force microscopy images of the micro-structured stamp and fluorescence image of the chemical pattern produced using this stamp.

Better mimetics of the cell membrane

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We present a new cell membrane mimicking platform and its in silico analogue called tethered bilayer lipid membrane (tBLM). We have characterized the tBLM formation process, from the initial intermolecular interactions in the lipid vesicle – surface contact zone to the resulting equilibrium tBLM, by employing the state-of-the-art molecular dynamics (MD) simulation and quartz crystal microbalance with dissipation monitoring (QCM-D). The detailed analysis of the process showed different molecular pathways of the interactions occurring in the contact (adsorption) zone of a small unilamellar vesicles (SUV) and the tether-terminated SAM. For the homogeneously distributed EG6AC8D tethers, the thermal motion was sufficient for their insertion into the adjacent lipid bilayer of the SUV. From the application point of view, the benefit of our tethering system is that the surface densities of the tethers as small as a few mol% are sufficient to reproducibly obtain stable tBLMs. The possibility to select from an optimal surface density and/or phase of the tethers can be important in designing tBLMs for efficiently mimicking different diffusion, transport and interaction phenomena occurring in the cell membrane, as well as for membrane protein incorporation. The presented platform is promising for quantitative biophysical studies as well as in pharmaceutical screening applications.

https://doi.org/10.1039/D2NR07069C

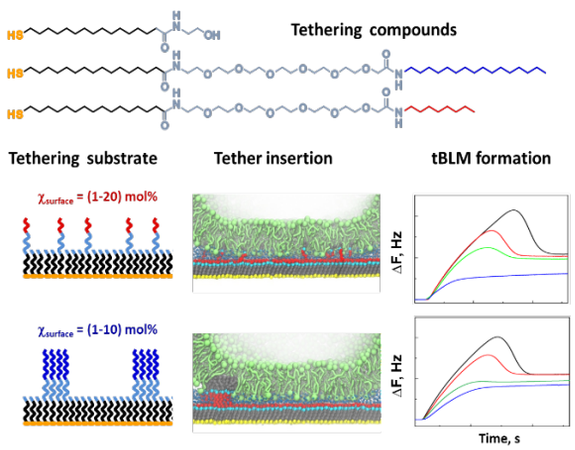
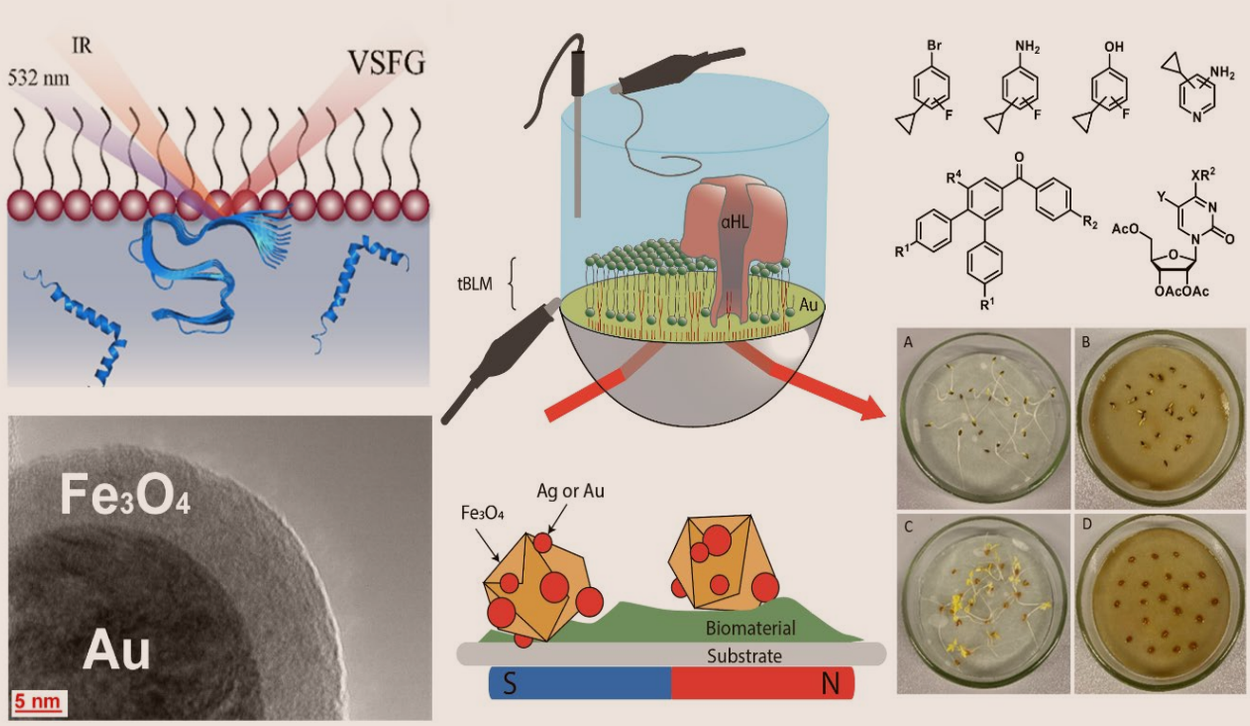


Fig. 2. (Top) Chemical structures of the compounds used for formation of supporting self-assembled monolayers on gold and for small unilamellar vesicles. (Bottom, left) Scheme of the surface structure. (Bottom, middle) The final snapshot after steered MD simulations plus 500 ns of relaxation. (Bottom, right) tBLM formation kinetics.



Department of Organic Chemistry

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Most of the essential processes in electrochemical catalysis, energy conversion, electrochemical and biochemical electron transfer, and biochemistry occur at the surfaces and interfaces. Understanding and predicting these processes requires detailed molecular-level insight into the surface-adsorbed species. Thus, our recent efforts were focused on using advanced spectroscopic techniques to investigate molecular adsorption, surface interactions, and electron transfer between adsorbed species and solutes. We utilized Raman, surface-enhanced Raman (SERS), and resonance Raman spectroscopies, integrated with electrochemistry, and advanced Raman methods based on dielectric shell-isolated plasmonic nanoparticles (SHINERS) and magneto-plasmonic nanoparticles. These methods were used to study the electrochemical potential-induced changes in the molecular structure of self-assembled monolayers, the structure of graphene-like materials, and biological materials, including living microbial cells and kidney cancerous tissues. Furthermore, vibrational sum-frequency generation (VSFG) spectroscopy was employed for the analysis of phospholipids at various deuteration levels. Recently, we adopted surface-enhanced infrared absorption spectroscopy (SEIRAS), which, due to its superb molecular sensitivity, allowed us to study water structure and lipid-protein interactions at the biomimetic lipid membrane constructs. Also, multiwavelength Raman spectroscopy, coupled with electrochemical techniques, has been effectively used to examine structural changes in electropolymerized conducting polymers during electron transfer. Furthermore, the organic synthesis group is developing and applying fundamental organic chemistry to optimize the synthesis of molecules required for research in biology, biochemistry, medicine, pharmaceutical and material sciences, physics, optoelectronics, semiconductors, etc. The synthesis of targeted molecules is optimized to provide high-quality products in an efficient and economical manner for the industrial and academic partners. The analytical group is mainly focused on the development, optimization, and validation of quantification methods using gas or liquid chromatography-mass spectrometry. Our research objectives encompass essential oils from Lithuanian plants, volatile

organic and bioactive compounds, and include collaborations with scientific institutes and private startups. Other area of our interest is the metrology in chemistry, accounting for precision and accuracy of measurement processes, and building of a new regional capacity for certification of reference materials according to the requirements of ISO 17034 standard. This multifaceted approach underscores our commitment to advancing scientific knowledge and technological capabilities in analytical chemistry.

Allelopathic Activity of Canadian Goldenrod Extracts on Seed Germination and Growth of Lettuce and Garden Pepper Cress

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Canadian goldenrod (*Solidago canadensis L.*), native to North America, has rapidly spread across Europe and other global regions, due to to its phenotypic plasticity, broad climatic tolerance, and effective propagation through seeds and rhizomes. The success in new environments is significantly influenced by allelochemicals, which impact seed germination, root formation, and overall growth of nearby flora. We evaluated the allelopathic effects of various *S. canadensis* extracts and essential oils on two model plants: lettuce (*Lactuca sativa L.*) and garden pepper cress (*Lepidium sativum L.*), comparing them to other *Solidago* species. Key findings include the potent inhibitory impact of aqueous flower extracts of all examined *Solidago* species on the model plants, with the Canadian goldenrod leaf water/diethyl ether extract showing particularly strong suppression at all tested concentrations. Notably, garden pepper cress exhibited greater susceptibility to Solidago spp. inhibitory effects compared to lettuce. Analysis of *S. canadensis* root essential oils, primarily composed of limonene and β-pinene, and inflorescence oils, containing α-pinene, germacrene D, limonene, and lupenyl acetate, revealed these components to be highly effective in inhibiting growth in both model plants. This comprehensive study underscores the allelopathic dominance of Canadian goldenrod and its potential implications on biodiversity in invaded ecosystems. The chemical composition of its extracts and essential oils, analyzed using advanced techniques like HPLC/DAD/TOF and GC/MS, provides valuable insights into the mechanisms behind its rapid spread and invasive success.

Canadian Goldenrod plant
(lt. Kanadinė rykštenė)

https://doi.org/10.3390/plants12071421

Nanoparticle-enhanced spectroscopic differentiation of cancerous tissues: a magneto-plasmonic approach

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Surface-enhanced Raman spectroscopy (SERS) has emerged as a crucial technique for detecting analytes at low concentrations. Enhancing the sensitivity and reproducibility of SERS signals, especially for cancer diagnosis, is a challenging task. The study presents a new technique for synthesizing Fe_3O_4@Ag nanoparticles by combining laser ablation with wet chemical methods. This strategy utilizes magnetic and plasmonic functionalities to achieve a homogenous nanoparticle distribution, eliminating the coffee-ring effect with an external magnetic field. Due to this, the variations in spectral intensity between different points were significantly reduced (cf. shaded areas in Fig. 1). Spectroscopic analysis of normal and cancerous human kidney tissue samples using NIR-range laser radiation revealed distinct spectroscopic signatures. Specific Raman shifts, notably at 480 and 853 cm^{-1}, were predominantly observed in cancerous tissues, corresponding to glycogen and lactose concentration changes. The data presented not only underscores the efficacy of MPNP-based SERS in discriminating malignant from non-malignant tissues but also propels this approach as a candidate for SERS-based cancer diagnostics.

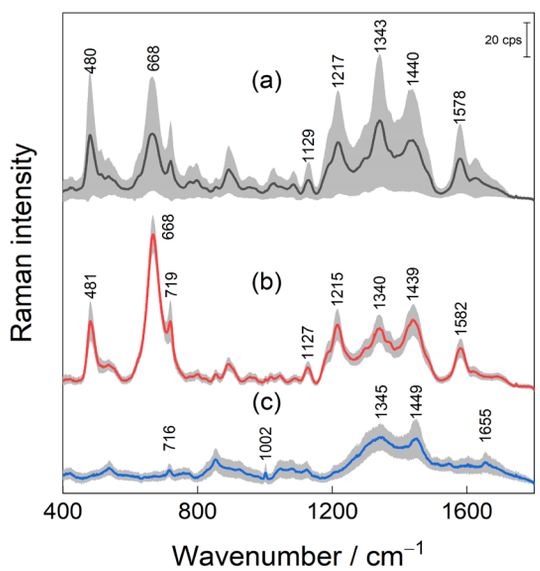

Fig. 1. SERS spectra from the cancerous kidney tissue utilizing (a) Ag and (b) Fe_3O_4@Ag nanoparticles. (c) Raman spectrum of the same sample. Shaded areas represent standard deviations from 100 measurements.

Enhancing gas chromatographic analysis: a novel cryo-enrichment module

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In this research, the application of cryo-enrichment in gas chromatography was explored. It is a technique designed to enhance the separation and sensitivity of the detection of volatile organic compounds in complex mixtures. By lowering the temperature of the chromatographic column to extremely low levels, this method reduces the volatility of compounds, leading to their efficient condensation onto the column's stationary phase. The primary focus of the research was the development of a custom cryo-enrichment module to improve system efficiency and sensitivity. Multiple prototypes were constructed and evaluated in-house, yielding significant improvements for gas chromatography. Notably, peak resolution increased up to 2.2 times, and the most optimal outcomes were achieved when cooling 95 cm of the column length, resulting in a 20-fold sensitivity boost. The limitations were related to the analyte working range, where some compounds were not retained adequately due to insufficient cooling, while others were retained excessively due to inadequate heating. The module was tested in method calibration, impurities analysis, fungicide analysis, and measuring terpenes in *Cannabis Sativa* biomass. We showed that cryo-enrichment in gas chromatography has a potential for improving analysis, but it also requires refinement and more practical applications.

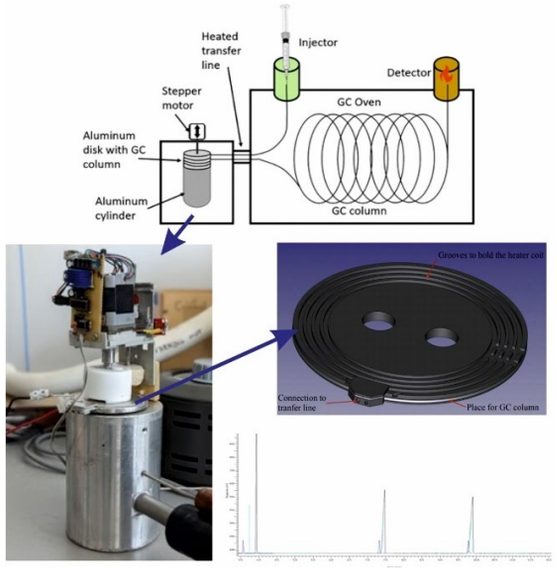

Fig. 2. Experimental setup of a custom cryo-enrichment module for gas chromatography demonstrating enhanced compound separation and system sensitivity.

https://doi.org/10.1093/chromsci/bmad079

Design of phosphine ligands for palladium-catalyzed reactions

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The requirement of fluorinated molecules has increased with their expanding applications in agriculture and pharmaceutical sciences. However, their availability is limited by harsh reactions usually needed for their preparation and/or functionalization in late-stage synthesis. Catalytic reactions can offer an efficient alternative. We use catalysis by design approach to develop new phosphine ligands suited for palladium (0/II) catalyzed cross coupling reactions. We also use computational methods (DFT) for pre-synthesis evaluation of energetic properties of potential catalytic system. The synthesis of ligand backbone has been modified to be feasible and safer on the larger scale. Further modification allows to control the steric and electronic properties of ligand needed for the successful targeted cross coupling reactions.

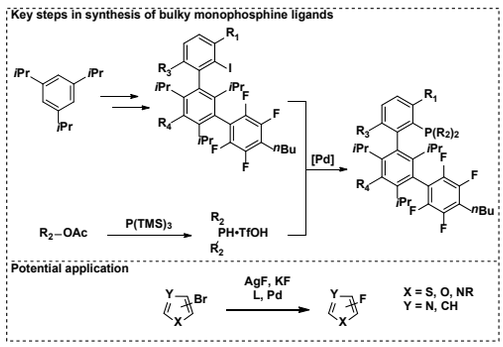

Fig. 3. Design and synthesis of phosphine ligands.

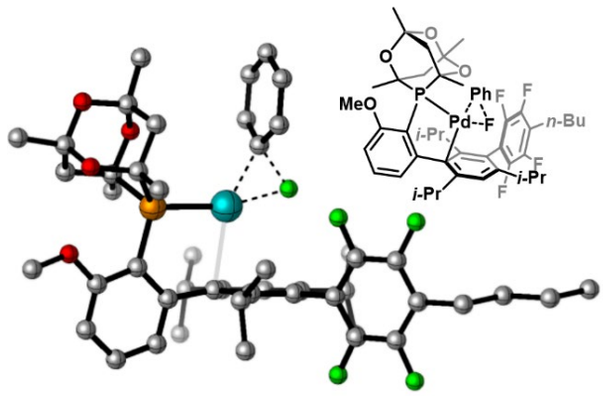

Fig. 4. Transition state of C–F reductive elimination from palladium (II) species.

Laser-ablated magneto-plasmonic nanoparticles: synthesis and spectroscopic applications

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We fabricate magneto-plasmonic nanoparticles via a 1064 nm picosecond-pulsed laser ablation of Fe/Au and Fe/Au/Fe composite thin films in acetone. Acetone is commonly used in nanomaterial synthesis because it solubilizes various metal precursors and provides a controlled environment for nanoparticle formation. The nanoparticles displayed a unique spherical core-shell (Au@Fe_3O_4) architecture. The combined plasmonic and magnetic features of these nanoparticles yield ultrahigh sensitivity in molecular detection enabled by the surface-enhanced Raman scattering, while their magnetic properties, attributed to the iron oxide shell, provide precise control over spatial positioning, vital for targeted therapies and diagnostics. The organic stabilizer-free nature and the inherent biocompatibility of the magnetic shell, coupled with the SERS activity of the plasmonic gold core, make these hybrid nanoparticles an excellent candidate for developing biosensors and broad biomedicine applications.

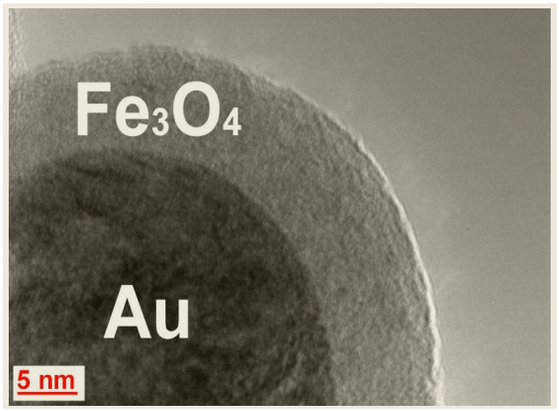
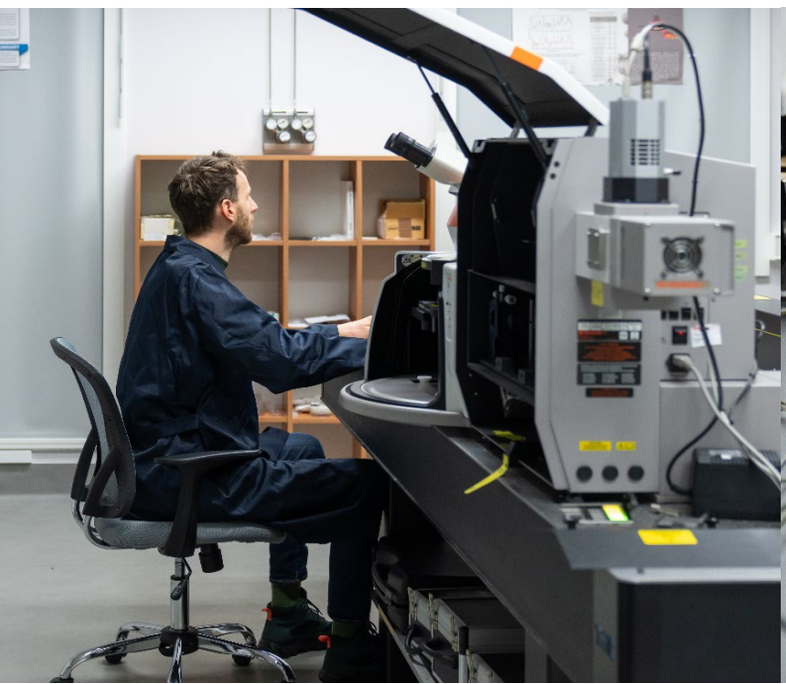
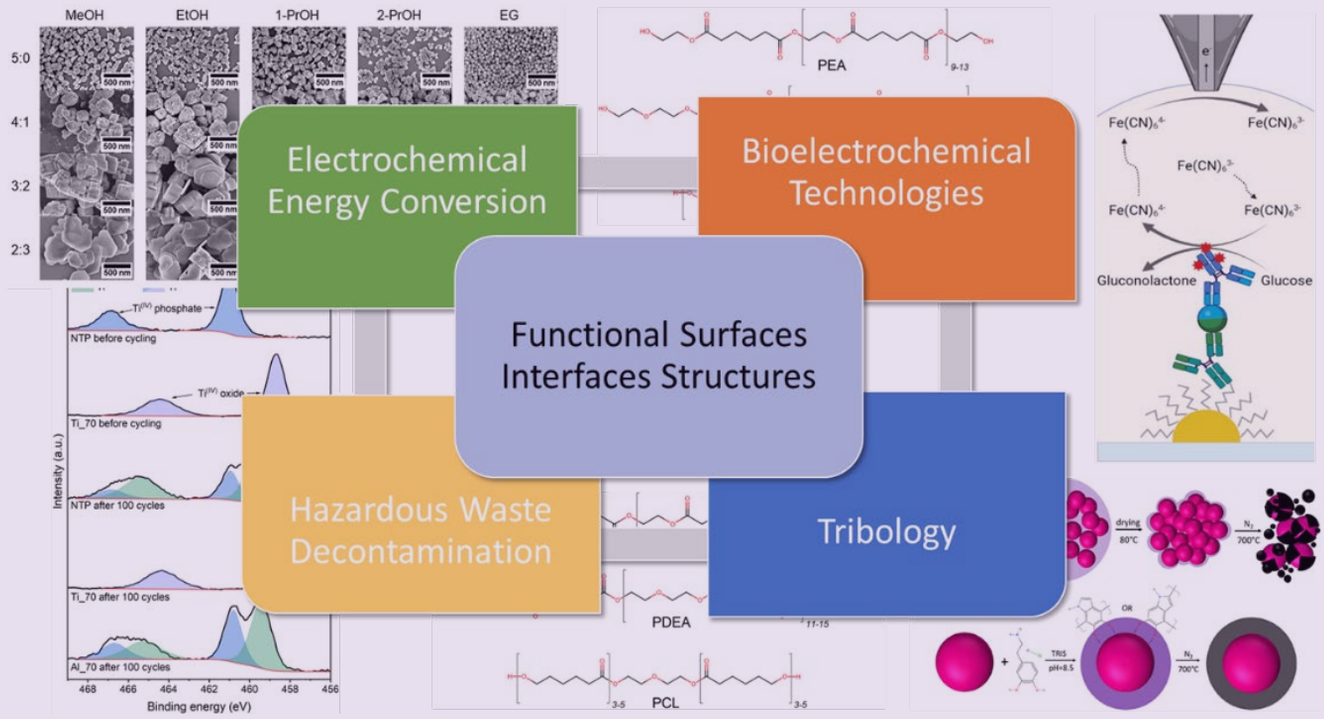


Fig. 5. Transmission electron microscopy image showing a close-up of the magneto-plasmonic Au@Fe_3O_4 nanoparticle.

https://doi.org/10.3390/coatings13091523





Department of Chemical Engineering and Technology

The main activities of the Department are primarily focused on the design and development of functional materials, active surfaces and interfaces for electrochemical energy conversion and circular economy. Four active Laboratories are currently operating within the Department: Electrochemical Energy Conversion, Tribology, Biolelectrochemical Technologies, and Hazardous Waste Decontamination. The extensive understanding and experience in electrochemistry and material science are the main driving forces for developing innovative sustainable technologies and new applications. The specific technologies currently developed in the Department are targeted towards the development of safe, sustainable and low-cost aqueous Na-ion batteries for stationary energy storage (NaAquaCell project), photoelectrochemical production of hydrogen and strong oxidants suitable for water treatment (CatWatSplit project), development of adhesives for recyclable multilayer packaging (TERMINUS project), and development of biological sensors and fuel cells. Environmental friendliness, sustainability, and circularity are imperative for all newly developed technologies and potential applications. The Department is also active in industrial scale up and applications of anodic aluminum coatings and metallization. A number of different characterization techniques are widely applied and developed with the emphasis on materials structural, morphological, and electrochemical properties.

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The use of reductive agents for developing capacity balanced aqueous sodium-ion batteries

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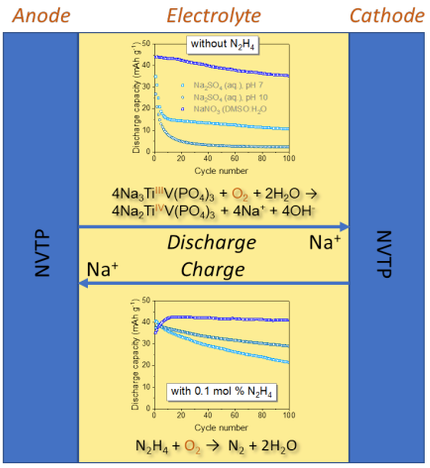
An aqueous symmetric $Na_2VTi(PO_4)_3$ | $Na_2VTi(PO_4)_3$ system was prepared and investigated as a model for electrolyte design and optimization with the aim of mitigating the main parasitic reactions in aqueous Na-ion batteries and making capacity balanced (N/P=1) battery cells. Oxygen reduction reaction is known to be the main parasitic process leading to self-discharge, Na-ion inventory loss, and material degradation in aqueous Na-ion batteries. We demonstrate that the introduction of a small concentration (ca. 0.1 mol%) of strongly reducing agent such as hydrazine into the aqueous or hybrid (e. g., water and dimethyl sulphoxide (DMSO)) electrolyte solutions chemically reduces dissolved oxygen and significantly improves the capacity retention of N/P=1 cells. Such low concentrations and the self-consuming nature of hydrazine in closed cells do not pose any health or chemical risks and present a viable strategy for practical cell design and applications. The N/P=1 cells are highly desired by battery industry due to the absence of deadweight, simpler design and lower materials and manufacturing costs. These results are applicable not only in the particular case of aqueous Na-ion batteries, but also useful in other aqueous battery chemistries, where such or similar parasitic processes play a significant role.



The introduction of a small concentration of strongly reducing agent such as hydrazine into purely aqueous or hybrid (water and dimethyl sulphoxide) electrolyte chemically reduces the dissolved oxygen and significantly improves the capacity retention of capacity balanced (N/P = 1) symmetric $Na_2VTi(PO_4)_3$ | $Na_2VTi(PO_4)_3$ cells during cycling.

https://doi.org/10.1002/batt.202300129
L. Vilciauskas, J. Juodkazyte, J. Pilipavicius, M. Petruleviciene, N. Traskina, Aqueous Electrochemical Energy Storage Cell And A Method For Manufacturing The Same, USPTO Application No. 18/150,857; Filing date: 01/06/2023.

The mechanism of $NaTi_2(PO_4)_3$ aqueous electrochemical degradation revisited

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Na SuperIonic CONductor (NASICON) structured materials attract increasing attention as electrodes for ion insertion batteries and deionization devices. $NaTi_2(PO_4)_3$ (NTP) is among the most suitable negative electrodes for aqueous electrolytes. However, various parasitic processes limit its Coulombic efficiency, self-discharge characteristics, and capacity retention. In this study, the degradation mechanisms of NTP in aqueous electrolytes were studied in great detail. The results obtained in specially designed electrochemical cells indicate that, to a different extent, both hydrogen evolution and oxygen reduction reactions are taking place during NTP electrochemical cycling and contribute to pH increase. The latter reaction due to the presence of $Ti^{(III)}$ species is found to be prevalent in aerated electrolytes. There is virtually no degradation and capacity loss observed at pH 7, but it becomes significant at pH 10 even in oxygen-free electrolytes. Contrary to previous studies, this work shows that capacity loss is actually slower at lower C-rates. The post mortem X-ray diffraction analysis shows that only a fraction of capacity loss could be directly attributed to NTP decomposition and even less to its dissolution into electrolyte. Most of the observed capacity fade is related to contact loss in the electrode structure which most likely comes from the formation of electron blocking aqueous interphasial layer.

https://doi.org/10.1016/j.electacta.2023.142993

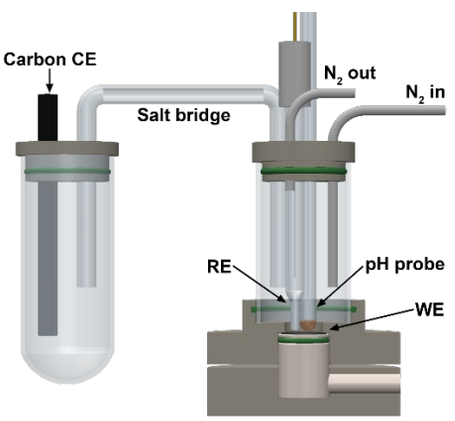

Fig. 1. Electrochemical measurement setup.

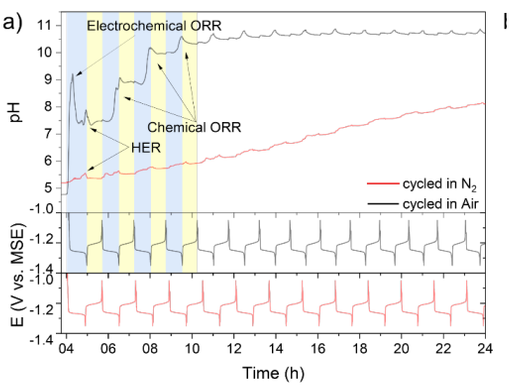

Fig. 2. Galvanostatic charge/discharge cycling results of NTP in naturally aerated and N_2 sparged 1 M Na_2SO_4 (aq.) electrolyte: local electrolyte pH and charge/discharge profiles.

Engineering of conformal electrode coatings by atomic layer deposition for aqueous Na-ion battery electrodes

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The application of atomic layer deposited layers directly on battery electrodes is an effective and viable approach for protecting the battery materials from degradation. Al_2O_3, TiO_2, and HfO_2 coatings are applied on $NaTi_2(PO_4)_3$, among the most studied negative electrode materials for aqueous Na-ion batteries. The coated electrodes are characterized in terms of electrochemical kinetics, charge capacity retention, and electrochemical impedance spectra. Al_2O_3, is shown to be insufficient to suppress parasitic processes and is eventually dissolved by reaction with hydroxide during extended cycling in aqueous Na_2SO_4. TiO_2 is found to be very resistant to increasing pH and remains almost intact during electrochemical cycling. However, we show that TiO_2 itself is electrochemically active in aqueous electrolytes at negative potentials. The protonation of TiO_2 leads to an additional increase in local pH which is detrimental to $NaTi_2(PO_4)_3$ and results in even faster capacity loss than in uncoated electrodes. HfO_2 is found to be highly stable and electrochemically inert for negative $NaTi_2(PO_4)_3$ electrodes operating in aqueous electrolytes.

DOI 10.1149/1945-7111/acd4ee

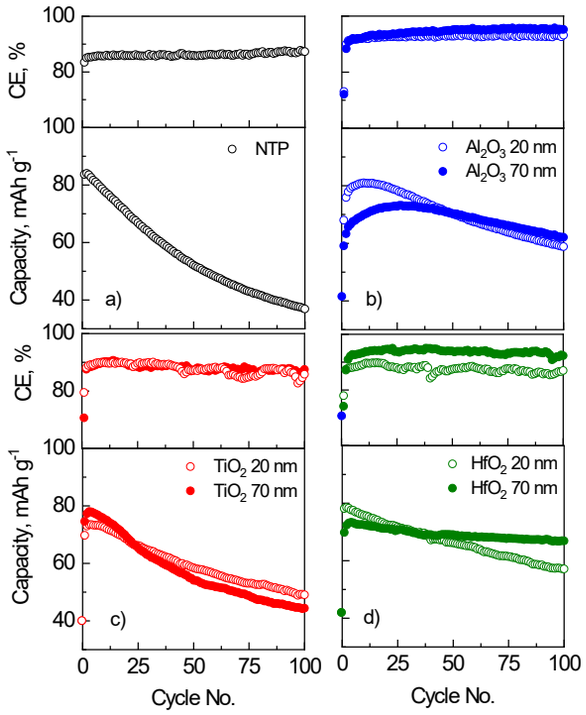

Fig. 3. Specific discharge capacity and Coulombic efficiency of (a) uncoated NTP, (b) Al_2O_3, (c) TiO_2 and (d) HfO_2-coated NTP electrodes during GCD cycling at 1C (0.133 A g^{-1}) rate in 1 M Na_2SO_4 (aq.) electrolyte.

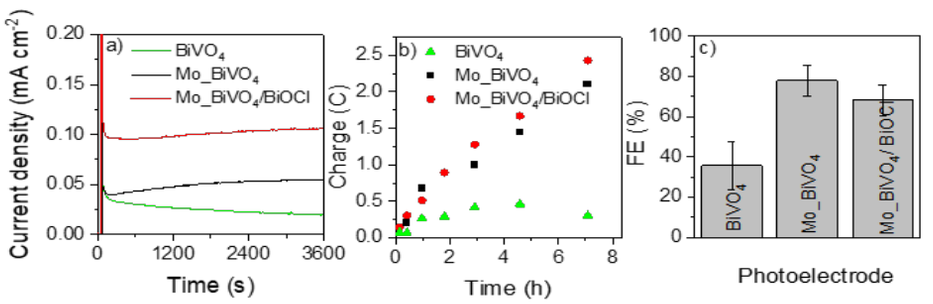

Fig. 4. (a) Variation of photocurrent during photoelectrolysis in 0.5 M NaCl solution at 1.4 V (vs. Pt) for $BiVO_4$ and 1.2 V (vs. Pt) for Mo_BiVO_4 and Mo_BiVO_4/ BiOCl; (b) correlation between cumulative duration of photoelectrolysis and charge passed through the cell for indicated photoelectrodes; (c) average Faradaic efficiency of PEC generation of ClO^- and ClO_2^-.

Optimization of $BiVO_4$ coatings for high yield photoelectrochemical production of reactive chlorine species

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Photoelectrochemical (PEC) synthesis of valuable chemicals, such as hydrogen and oxidants, is widely studied as a potential alternative to replace conventional synthesis processes with high carbon footprint. In this study two different approaches were used to improve photoelectrochemical activity of $BiVO_4$ coatings, i.e. doping with molybdenum and heterostructuring with BiOCl. Performance of the photoelectrodes was tested in the solutions of Na_2SO_4 and NaCl. PEC activity was found to increase in the sequence $BiVO_4$ < Mo_BiVO_4 < Mo_BiVO_4/BiOCl and the enhancement was much more pronounced in chloride medium. Mo doping was found to double the incident photon to current conversion efficiency (from 5% to 10%) as well as Faradaic efficiency of the photoinduced generation of reactive chlorine species, i.e. ClO^- and ClO_2^- (from an average of 36% to 78%). Construction of a heterojunction between Mo_BiVO_4 and BiOCl promoted separation of photogenerated electrons and holes and led to a significant enhancement of photocurrent. The presence of BiOCl layer was found to catalyze photooxidation of ClO^- to ClO_2^-. The findings of the study demonstrate the potential of $BiVO_4$-based coatings for PEC production of oxidants via saline water splitting.

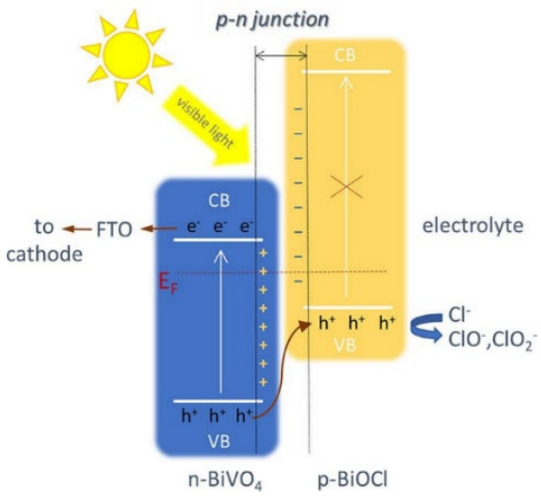

Fig. 5. Schematic representation of the photoinduced charge separation and transfer processes in n-type $BiVO_4$ and p-type BiOCl heterostructure.

https://doi.org/10.1016/j.jphotochem.2023.114842

Scanning electrochemical microscopy: Glucose oxidase as an electrochemical label in sandwich format immunoassay

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An electrochemical sandwich immunoassay for the detection of human growth hormone (hGH) using scanning electrochemical microscopy (SECM) on an array of 30 µm diameter gold micro-discs (Au) was proposed. The Au was modified with a self-assembled monolayer (SAM), on which we covalently immobilized monoclonal antibodies against hGH (m-anti-hGH). After the hGH was captured by the m-anti-hGH, polyclonal detection antibodies conjugated with glucose oxidase (p-anti-hGH-GOx) interacted with the captured hGH, forming sandwich type immune complexes (Au-SAM/m-anti-hGH/hGH/p-anti-hGH-GOx). GOx activity (which is proportional to the p-anti-hGH-GOx presence) was registered using potassium hexacyanoferrate(III) as a redox mediator. It was shown that hGH concentrations as low as 40 nM could be detected by SECM. The flux of the redox mediator from the Au with formed sandwich type immune complexes after the addition of glucose was calculated using a mathematical model and the generation rate of $[Fe(CN)_6]^{4-}$ in the presence of glucose was estimated to be 28 pmol s^{-1} cm^{-2}. Thus, GOx was successfully applied as an electrochemical label for detecting hGH in a sandwich type immunoassay by SECM operating in SG/TC mode. The methodology described herein could be adapted for the electrochemical detection of many other antigens of interest.

https://doi.org/10.1016/j.electacta.2023.142790

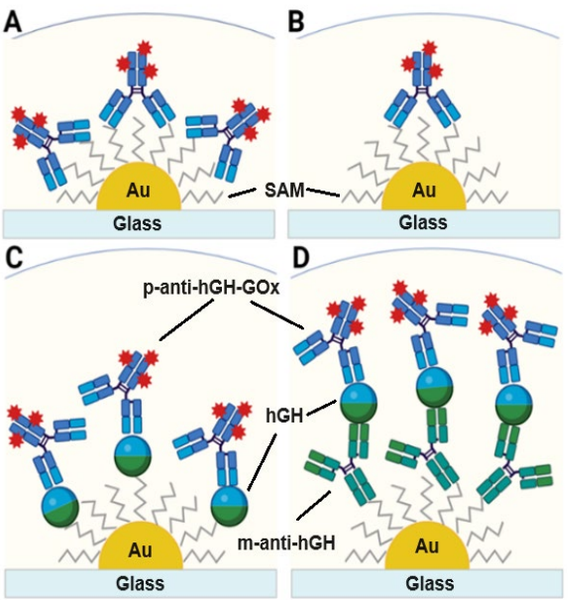


Fig. 6. Schematic representation of different samples. (A) Au-SAM/p-anti-hGH-GOx 100 nM; (B) Au-SAM/p-anti-hGH-GOx 10 nM; (C) Au-SAM/hGH/p-anti-hGH-GOx; (D) Au-SAM/m-anti-hGH/hGH/p-anti-hGH-GOx.

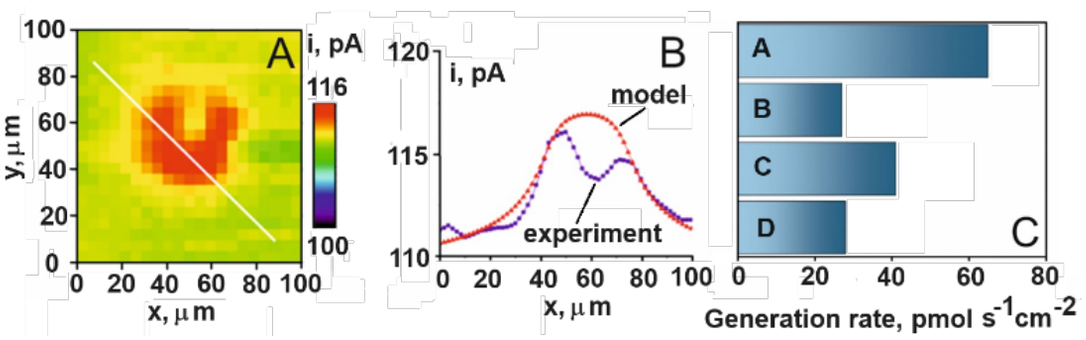
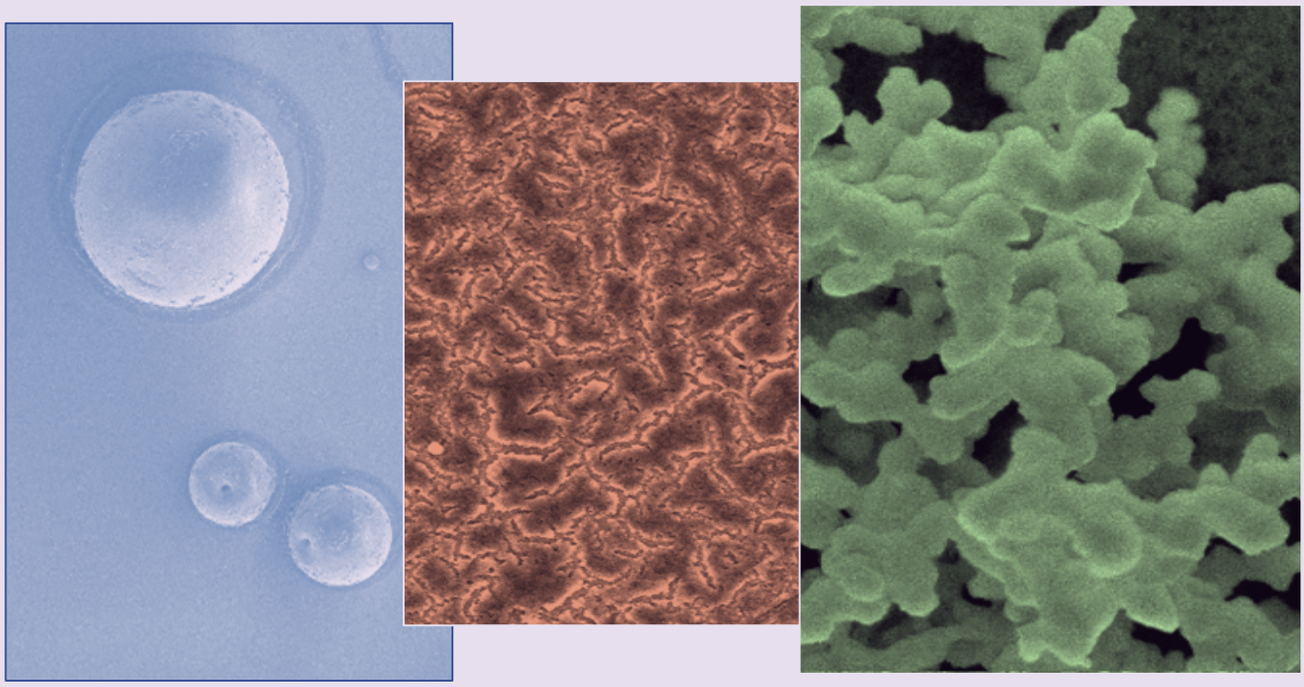


Fig. 7. (A) SECM image recorded over sandwich-type immune complex. (B) Cross section profile extracted from SECM image. (C) The flux values of $[Fe(CN)_6]^{4-}$ obtained by fitting the extracted profiles from samples in Fig 6.



Department of Electrochemical Material Science

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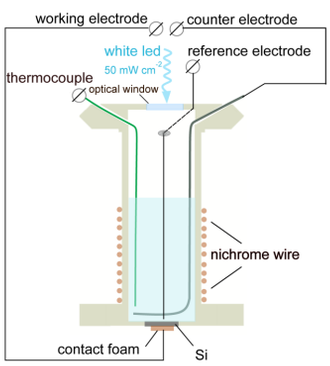
The research activities of the Electrochemical Materials Science Division focus on the application of electrochemical methods and processes to the development and characterization of new materials and technologies for energy conversion, photocatalysis and nanomedicine. The main R&D activities include but are not limited to:

- Silicon electrochemistry. Electrochemical synthesis of nano/microstructures and their application in sustainable energy: photovoltaics, hydrogen photogeneration, new generation batteries.
- Development of new nanomaterials and their application in optoelectronics, materials engineering, energy conversion.
- Electrochemical deposition of transparent and/or electrically conductive nanothin semiconductor layers for photo/electrocatalytic reactions.
- Search for synthesis methods of new superparamagnetic and luminescent nanoparticles, their characterization and investigation of their possible use in nanomedicine.
- Investigation of the processes of nanostructured titania and iron oxide layers formation, modification of their composition and surface functionalization.
- Testing of corrosion resistance of metals for industrial applications in the accredited Corrosion Research Laboratory. Development of materials and methods for corrosion protection.



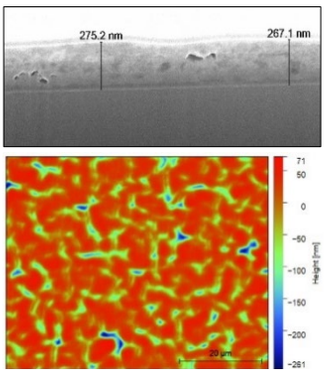
The photoelectrochemical cell for the deposition of Si–C coatings in ionic liquid.

A new technology of photoelectrochemical deposition of silicon-carbon layer from an ionic liquid electrolyte

In recent year a new technology of photoelectrochemical deposition of silicon-carbon layer from an ionic liquid electrolyte was developed. An advantage of p-type semiconductors to generate the photoelectrons was applied to photoelec-trochemically

deposit Si and Si–C structures. Nano-layers have been deposited from the electrolyte composed of N-trymethyl-N-hexy-lamonium (TMHA), bis(trifluoromethylsulfo-nyl)amide (TFSA) and silicon tetrachloride ($SiCl_4$) as a silicon precursor. The nanostructures were deposited on p-Si, p-GaAs as well as aluminum alloy AA 2024 substrates. Semiconductors were activated using white LED illumination and the structures in the far region of cathodic potentials were deposited, where the decomposition of the ionic liquid occurs. The deposition was achieved at nearly room temperature (40 °C). Amorphous Si–C layers with micrometer-sized carbon inclusions in the silicon were formed. The produced layers were photo-responsive as proven by the light-enhanced cathodic currents measured on an optically inactive electrode made of AA 2024 alloy. The proposed method paves the way for the electrochemical modification of semiconductors and metals with Si and Si–C structures, which are applicable in various fields, such as batteries, anti-corrosion coatings, photovoltaics, or photoelectrochemical electrodes for hydrogen production.

This research was funded by the Lithuanian Scientific Council under project agreement S-MIP-21-124.



Cross section and surface profile of the deposited Si-C composite coating.

https://doi.org/10.3390/coatings13071159.
Patent application LT2023 519; No 107957 is pending

Magnetic nanoparticles decorated with gold nanoclusters – applications in cancer theranostics

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This study is devoted to the synthesis of luminescent magnetic nanoparticles (Nps) by conjugation with gold nanoclusters (NCs), which possess both magnetic resonance and optical biopsy properties. The designed Nps are novel, non-toxic, stable for months, accumulate in cells and induce cell death upon exposure to visible light.

https://doi.org/10.1002/admi.202300462

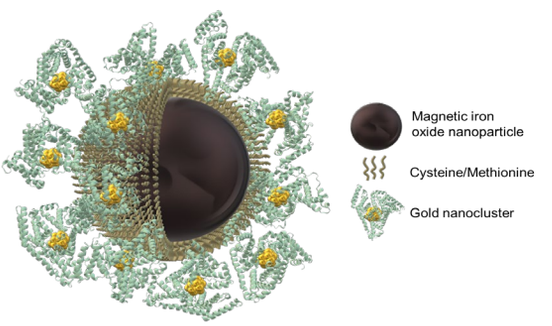

Fig. 1. Suggested model for magnetic Np conjugated with gold NCs.

Aluminum anodizing in an aqueous solution of formic acid with ammonium heptamolybdate additive

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Aluminum oxide films containing a high content of entrapped carbon species throughout the film thickness have been fabricated by anodizing aluminum in an aqueous solution of formic acid and ammonium heptamolybdate at 60 to 80 V. The unique morphology, composition and formation mechanism have been studied by numerous techniques and discussed.

https://doi.org/10.1149/1945-7111/acb019

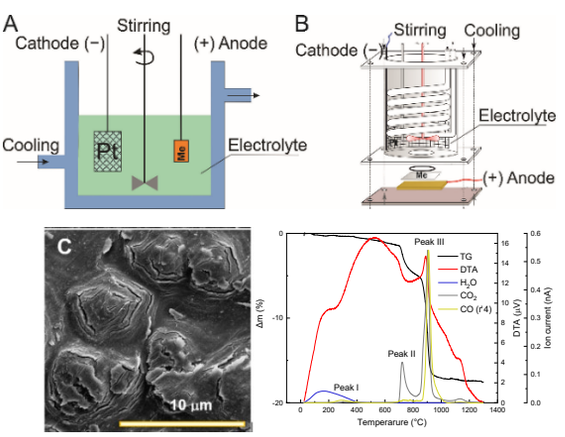

Fig. 2. (A,B) Al anodizing schemes, (C) surface morphology, and (D) TG/DTA plots for hybrid-type aluminum oxide/carbon film.

Composite p-Si/Al_2O_3/Ni photoelectrode for hydrogen evolution reaction

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A photoelectrode for hydrogen evolution reaction (HER) is proposed, which is based on p-type silicon (p-Si) passivated with an ultrathin (10 nm) alumina (Al2O3) layer formed using atomic layer deposition (ALD) and modified with microformations of a nickel catalyst. The Ni catalyst increased the HER rate up to one order of magnitude, which was comparable with the rate measured on a hydrogen terminated electrode. The properties of the alumina film on silicon were comprehensively studied.

https://doi.org/10.3390/ma16072785

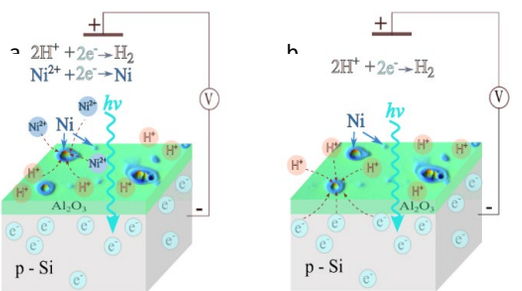
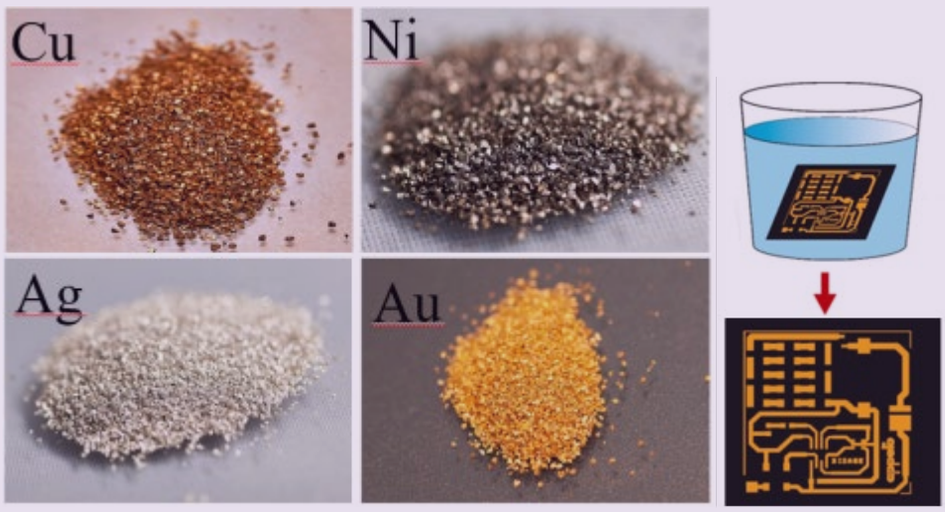
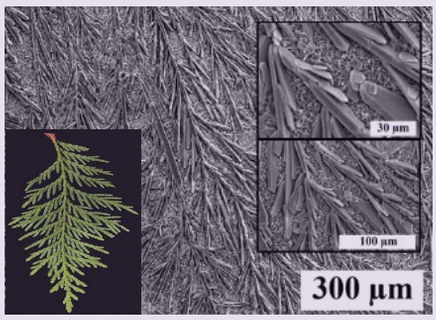
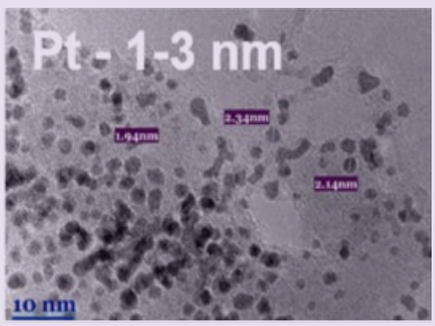


Fig. 3. (a) Schematic representation of Ni^{2+} deposition and (b) H+ reduction at Ni micro-catalyst by the photoelectrons induced in p-Si-Al_2O_3 electrode.





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



Department of Catalysis

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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. The autocatalytic metal ion reduction systems are widely used for decorative and functional purposes or selective metallization, i. e. for deposition of a conductive metal layer on plastics, polyester fabric, silicon carbide or quartz particles, dielectrics, semiconductors, or conductors with a complicated configuration without external current. The selection of suitable reducing agents and conditions of the reaction (temperature, the 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 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 different surfaces (titanium, copper, nickel or copper foams, carbon, graphene powder, N-doped carbon from biowaste or other supports) with enhanced activity towards the oxidation of various fuels, have been developed. The obtained catalysts are promising anode materials and can be used in practical fuel cells.

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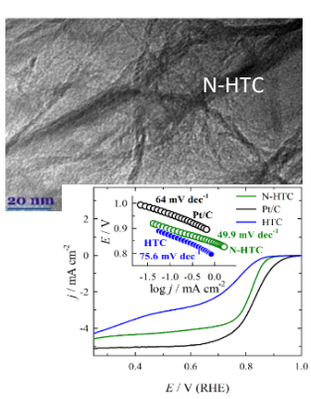
Synthesis of nitrogen-doped carbon catalyst from hydrothermally carbonized wood chips for oxygen reduction

An efficient carbon material was prepared using hydrothermal carbonization (HTC) of birch-wood chips in the water under elevated pressure, subsequent chemical activation and doping with nitrogen. The obtained catalyst had a large specific surface area of 2431 $m^2\ g^{-1}$ and a high nitrogen content of 4.60 at.%. Most of the nitrogen was in the pyridinic-N (57.61 at.%) form. The synthesized material exhibits excellent electro-catalytic activity for the oxygen reduction reaction with an



onset potential of 0.9 V versus the reversible hydrogen electrode, showing the 4e⁻ electrons transfer path in 0.1 M KOH solution. This work demonstrates an efficient and sustainable approach to developing green energy-related material while considering biorefinery concepts. The synthesized excellent N-HTC material is a promising alternative to state-of-the-art precious metal-based catalysts for fuel cells, metal-air batteries, etc.

https://doi.org/10.1016/j.catcom.2023.106797

Copper-nitrogen dual-doped activated carbon derived from alder wood as an electrocatalyst for oxygen reduction

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This study deals with the facile synthesis of inexpensive wood-derived nanocarbon-based catalyst materials, which can achieve the goals of a low carbon economy, e. g. by replacing platinum in low-temperature fuel cells. Moreover, combining metal nanoparticles and wood-derived nitrogen-doped nanocarbon-based materials provides a new opportunity to design next-generation catalysts. Modifying the N-doped activated carbon with Cu nanoparticles resulted in a higher oxygen-reduction activity than that of a pure N-doped carbon.

https://doi.org/10.1016/j.catcom.2023.106743

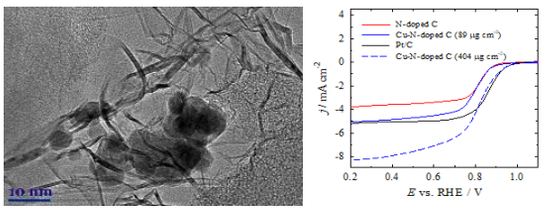

Fig. 1. TEM view and linear sweep voltometry (LSV) curves for oxygen-reduction reaction (ORR) recorded on N-doped C, Pt/C, and Cu-N-doped C at 1600 rpm in O_2-saturated 0.1 M KOH at 10 mV s^{-1}.

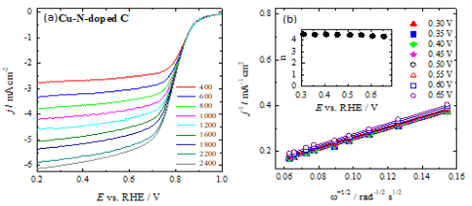

Fig. 2. (a) LSV curves for ORR on Cu–N-doped C in 0.1 M KOH at different rpm at 10 mV s^{-1}. (b) K–L plots derived from the RDE data.

Bimetallic 3D nickel-manganese/titanium bifunctional electrocatalysts for efficient hydrogen and oxygen evolution reaction in alkaline and acidic media

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A set of self-supported bimetallic NiMn alloy catalysts with a unique 3D porous architecture and various Ni:Mn molar ratios have been successfully synthesized through the electrochemical deposition technique. The electrochemical performance results of NiMn for hydrogen and oxygen evolution (HER and OER) reactions manifested that the amalgamation of the Mn element with Ni remarkably enhanced the electrocatalytic activity of the catalysts for HER and OER.

https://doi.org/10.3390/coatings13061102

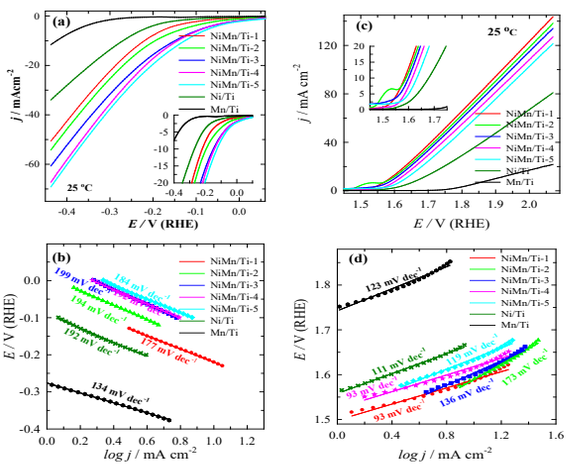

Fig. 1. HER (a) and OER (c) LSVs recorded in 1 M KOH at 10 mV s^{-1}. (b,d) The coresponded Tafel slopes.

Investigation of hydrogen and oxygen evolution on cobalt-nanoparticles-supported graphitic carbon nitride

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This study focuses on fabricating cobalt particles deposited on graphitic carbon nitride (Co/gCN) using annealing, microwave-assisted, and hydrothermal syntheses and their employment in HER and OER reactions. The catalyst prepared via the annealing of $Co(NO_3)_2$ with melamine exhibited the highest activity and gave the lowest overpotentials for HER and OER compared to the other Co-supported gCN catalysts prepared via microwave-assisted and hydrothermal syntheses. Notably, the annealing treatment of $Co(NO_3)_2$ with melamine is a potential method for its practical applications in electrochemical water splitting.

https://doi.org/10.3390/ma16175923

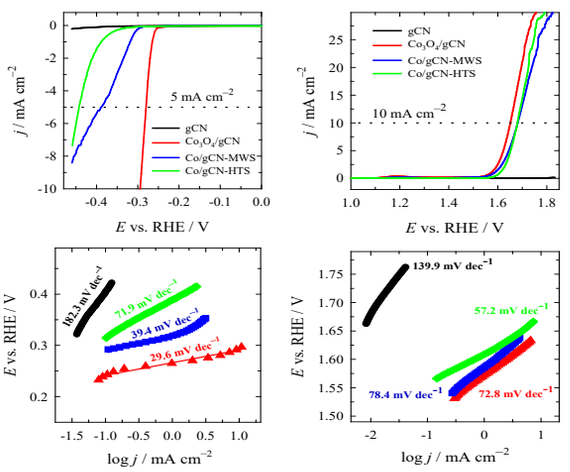
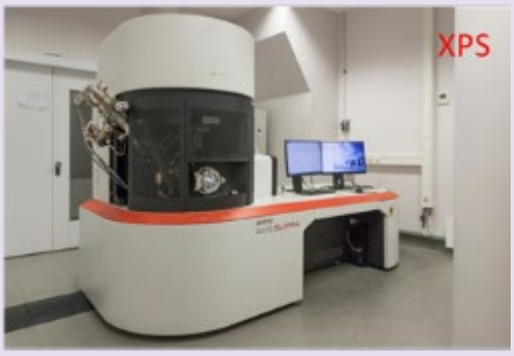
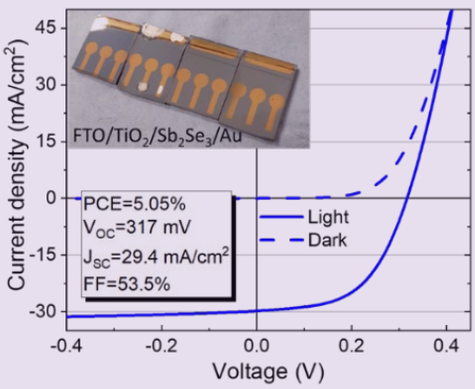


Fig. 2. HER (a) and OER (b) LSVs of gCN, Co_3O_4/gCN, Co/gCN-MWS, and Co/gCN-HTS in 1 M KOH at 2 mV s^{-1}. (c,d) The coresponded Tafel slopes.





Department of Characterisation of Materials Structure

Department is divided into two laboratories: the research area of the Laboratory of Characterisation of Material Structure is focused on the in-depth characterisation of materials structure by various microscopic and spectroscopic methods. Our goal is to provide a comprehensive analysis of materials crystalline structure, morphology, chemical and phase compositions. Research field of the Laboratory for photoelectric Materials entails the synthesis and study of the chalcogenide materials for optoelectronic application with a special focus on the development of sustainable thin film solar cells. The objective is to develop chalcogenide-based wide and narrow bandgap technologies for application in flexible, indoor, semi-transparent and multijunction solar devices.

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Band gap engineering by cationic substitution in $Sn(Zr_{1-x}Ti_x)Se_3$ alloy for bottom sub-cell application in solar cells

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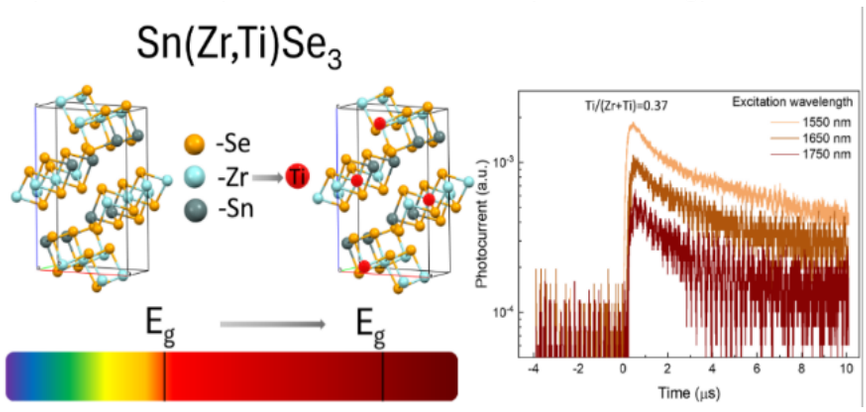
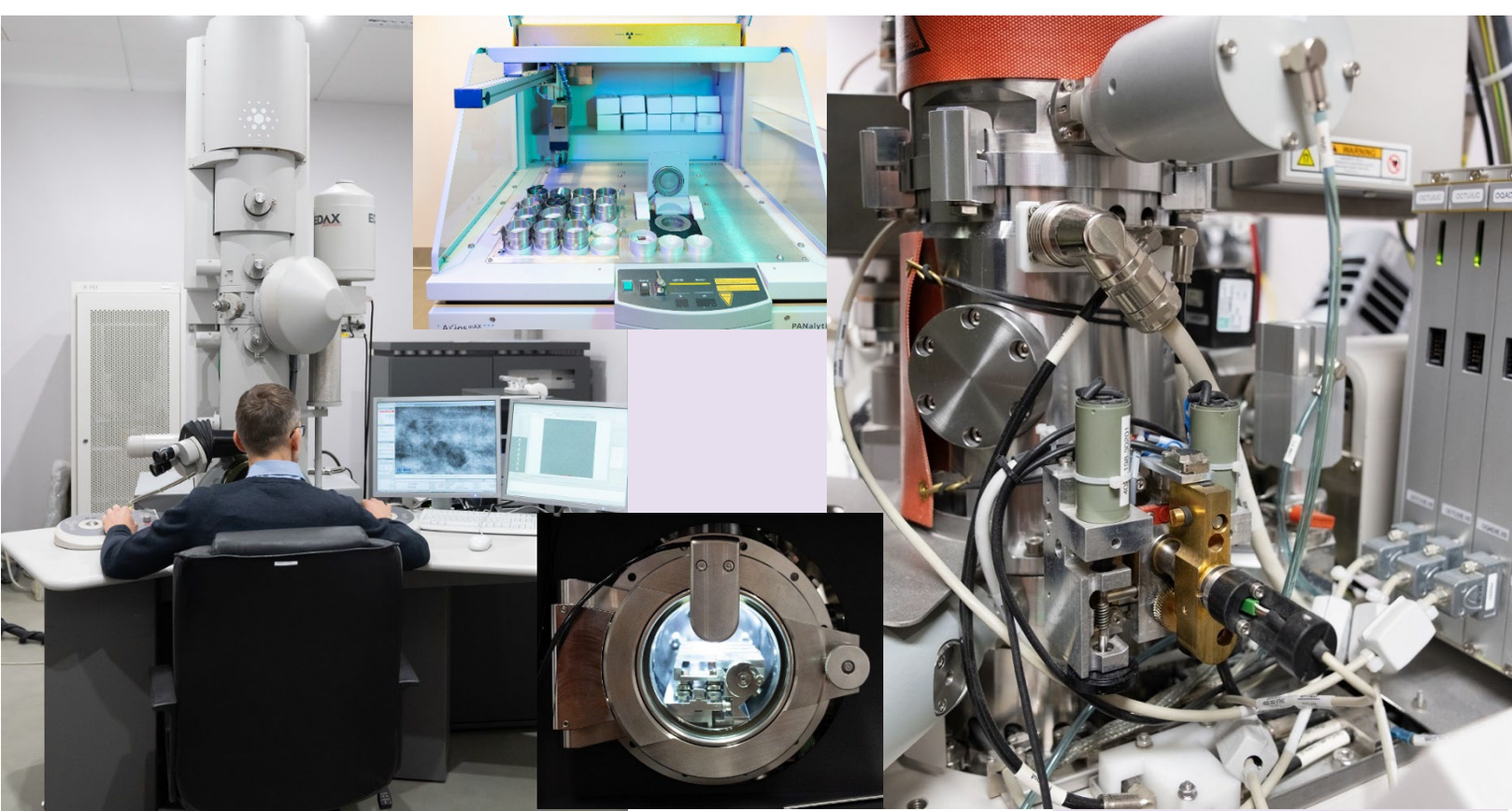
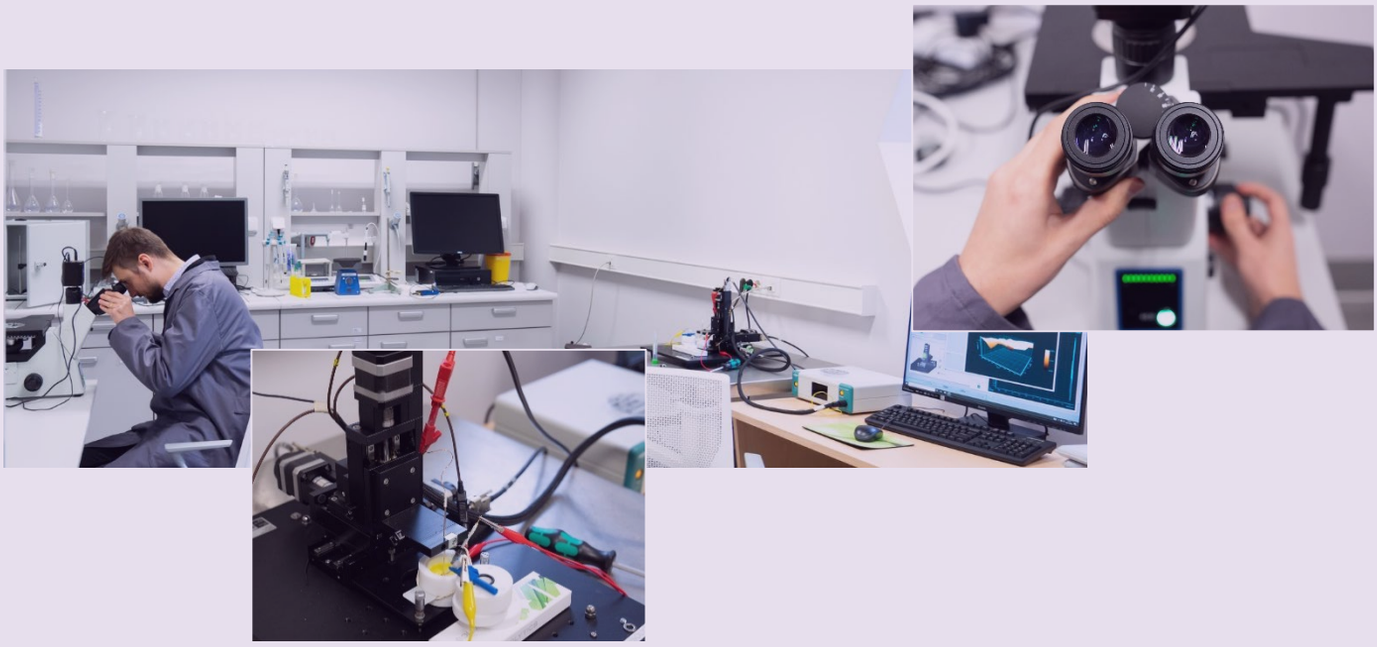
Next-generation solar cells employ multiple junctions to push power conversion efficiency beyond the Shockley–Queisser limit. As the tandem devices based on c-Si and wide band gap absorbers are showing impressive performances, introducing a third junction can boost efficiency even further. In this work, a novel material was synthesized and studied with the potential to harvest the infrared part of the solar spectrum that is not utilized by c-Si technology. The research team employed a solid-state synthesis method to produce $Sn(Zr,Ti)Se_3$ crystals with various Zr/Ti ratios and studied their optical and electrical properties. The authors found that $Sn(Zr_{1-x},Ti_x)Se_3$ alloys crystallised in a needle-like phase and were stable up to x=0.44. With increasing concentration of Ti, the band gap of $Sn(Zr_{1-x},Ti_x)Se_3$ redshifted reaching 0.78 eV which was near the optimum value required to reach maximum efficiency of infrared solar cells.



The Bandgap of $SnZrSe_3$ was successfully engineered by cationic substitution to create novel materials photoactive in short wavelength infrared region.

https://doi.org/10.1039/D3TA05550G





Department of Nanotechnology

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The main research directions of the Department of Nanotechnology are related to developing sensors, biosensors, immuno-analytical systems, molecularly imprinted polymer-based sensors, and related research. A significant part of the experiments is dedicated to developing optical, acoustic, and electrochemical sensors for detecting SARS-CoV-2 proteins. The optical and acoustic biological sensors are studied by spectroscopic ellipsometry and quartz crystal microbalance methods. To gain sensitivity to SARS-CoV-2 proteins, the electrochemical sensors are modified with self-assembled monolayers or conducting polymers, including molecularly imprinted polymers. These sensors are studied by differential pulse voltammetry, cyclic voltammetry, pulsed amperometric detection, and other electrochemical methods.

Study of SARS-CoV-2 spike protein wild-type and the variants of concern real-time interactions with monoclonal antibodies and convalescent human serum

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The spike (S) protein and its receptor-binding domain (RBD) of the coronavirus SARS-CoV-2 have been continually evolving, yielding the majority of significant missense mutations and new variants of concern. In this study, we examined how monoclonal antibodies against RBD (mAbs-SCoV2-RBD) and polyclonal antibodies present in convalescent human serum specifically interact with the S protein of wild-type and SARS-CoV-2 variants of concern (VOCs) in real-time and how this can be reflected through surface mass density. Moreover, we combined two distinct, label-free measurement techniques: one based on changes in surface electromagnetic waves after reflection from the surface, and the other on changes in acoustic waves. The results of this study can give insights into the differences between the interaction of monoclonal and polyclonal antibodies with SARS-CoV-2 VOCs.

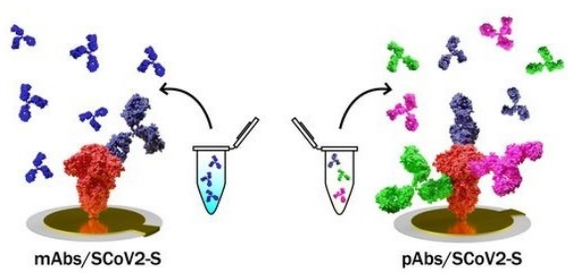

Fig. 1. Scheme of SARS-CoV-2 spike protein wild-type and the variants of interaction with monoclonal antibodies.

https://doi.org/10.3390/bios13080784

Revealing the SARS-CoV-2 spike protein and specific antibody immune complex formation mechanism for precise evaluation of antibody affinity

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The profound understanding and detailed evaluation of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) spike (SCoV2-S) protein and specific antibody interaction mechanism is of high importance in the development of immunosensors for COVID-19. In the present work, we studied a model system of immobilized SCoV2-S protein and specific monoclonal antibodies by molecular dynamics of immune complex formation in real-time. We simultaneously applied spectroscopic ellipsometry and quartz crystal microbalance with dissipation to reveal the features and steps of the immune complex formation. We showed direct experimental evidence based on acoustic and optical measurements that the immune complex between covalently immobilized SCoV2-S and specific monoclonal antibodies is formed in two stages. The reported findings can facilitate a deeper understanding of antigen-antibody immune complex formation steps and can open a new way for the evaluation of antibody affinity towards corresponding antigens.

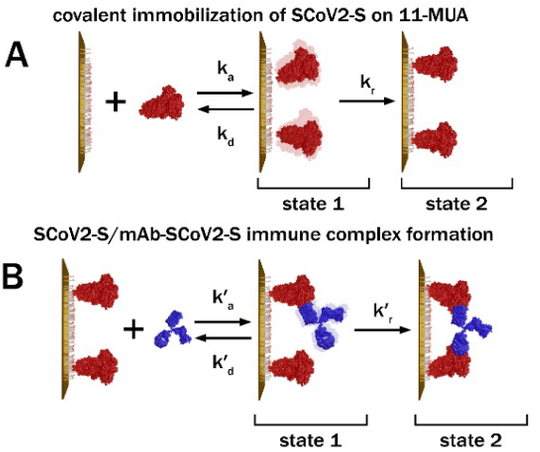

Fig. 2. Schematic representations of the two-step model of SCoV2-S covalent immobilization (A) and affinity-based interaction between covalently immobilized SCoV2-S and mAb-SCoV2-S (B). The proteins enter the initial state 1 at a rate constant ka, then may desorb at a rate constant—k_d or bind strongly at a rate constant—k_r.

https://doi.org/10.3390/ijms241713220

Development of essential oil delivery systems by 'click chemistry' methods: possible ways to manage Duchenne Muscular Dystrophy

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Duchenne muscular dystrophy (DMD) is a rare, severe, progressive, muscle-wasting disease. Today, the therapeutic standard for treating DMD is corticosteroids, which cause serious adverse side effects. Nutraceuticals, e.g., herbal extracts or essential oils (EOs), are possible active substances to develop new drug delivery systems to improve DMD patients lives. Herbal extracts and EOs combined with click chemistry can lead to the development of safer treatments for DMD. In this review, we focus on the need for novel drug delivery systems using EOs as the therapy for DMD and the potential use of click chemistry for drug delivery systems. New EO complex drug delivery systems may offer a new approach to improving

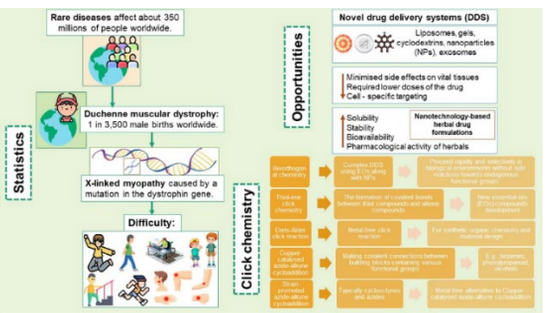

Fig. 3. Opportunities of novel drug delivery systems to treat Duchenne muscular dystrophy.

muscle conditions and mental health issues associated with DMD. However, further research should identify the potential of these systems in the context of DMD. In this review, we discuss possibilities for applying EOs to DMD before implementing expensive research.

https://doi.org/10.3390/ma16196537

Electrochemical biosensor for the determination of specific antibodies against SARS-CoV-2 spike protein

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In this article, we report the development of an electrochemical biosensor for the determination of the SARS-CoV-2 spike protein (rS). A gold disc electrode was electrochemically modified to form the nanocrystalline gold structure on the surface. It was further altered by a self-assembling monolayer based on a mixture of two alkane thiols: 11-mercaptoundecanoic acid (11-MUA) and 6-mercapto-1-hexanol (6-MCOH) (SAM_{mix}). This electrode was used to design an electrochemical sensor suitable for determining antibodies against the SARS-CoV-2 rS protein (anti-rS). We assessed the association between the immobilized rS protein and the anti-rS antibody present in the blood serum of a SARS-CoV-2 infected person using three electrochemical methods: cyclic voltammetry, differential pulse voltammetry,

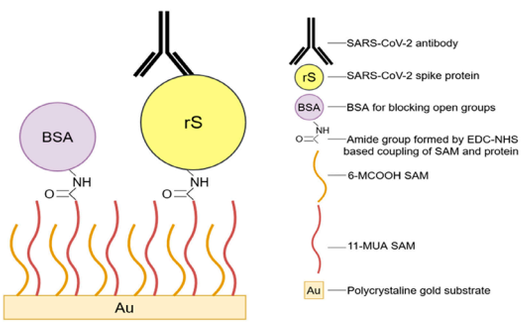

Fig. 4. The layered composition of the electrochemical biosensor based on the gold electrode modified with a SAM_{mix} and covalently immobilized spike protein used for the detection of anti-rS antibodies.

and potential pulsed amperometry. We demonstrated that the latter two methods display similar sensitivity.

https://doi.org/10.3390/ijms24010718

Molecularly imprinted polymers for the recognition of biomarkers of certain neurodegenerative diseases

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The appearance of the biomarkers in body fluids like blood, urine, saliva, tears, etc. can be used for the identification of many diseases. This article aims to summarize the studies of electrochemical biosensors with molecularly imprinted polymers (MIPs) as sensitive and selective layers on the electrode to detect protein-based biomarkers of such neurodegenerative diseases as Alzheimer and Parkinson diseases and stress. We focus on the detection methods based on amyloid-ß oligomers and p-Tau, which are representative biomarkers for Alzheimer disease, α-synuclein as the biomarker of Parkinson disease, and α-amylase and lysozyme as the biomarkers of stress using molecular imprinting technology. The research methods, the application of different electrodes, the influence of the polymers, and the established detection limits are reviewed and compared.

https://doi.org/10.1016/j.jpba.2023.115343

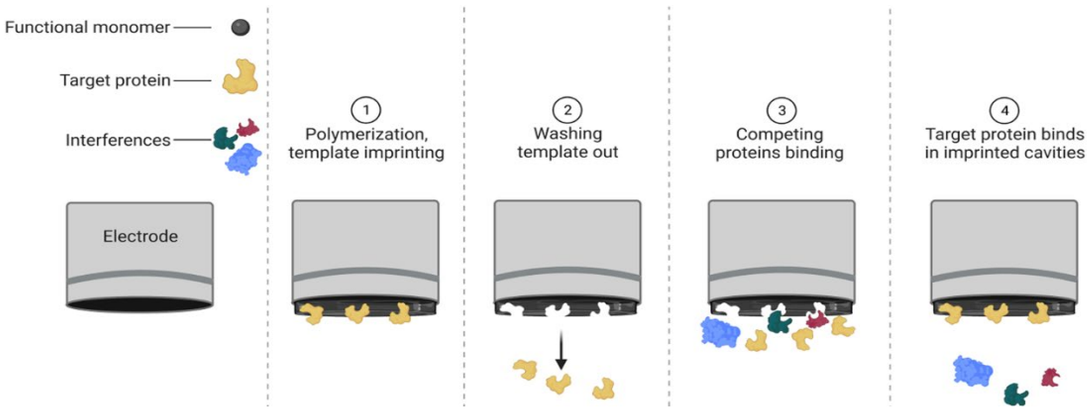

Fig. 5. An illustration of the MIP preparation principles.

Polyaniline-based electrochemical immunosensor for the determination of antibodies against SARS-CoV-2 spike protein

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We present an impedimetric system for the detection of antibodies against severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) Spike protein. The sensing platform is based on recombinant Spike protein (SCoV2-rS) immobilized on the phytic acid-doped polyaniline films (PANI-PA). The affinity interaction between immobilized SCoV2-rS protein and antibodies in the physiological range of concentrations was registered by electrochemical impedance spectroscopy. Analytical parameters of the sensing platform were tuned by variation of electro-polymerization time during PANI-PA films synthesis. The presented sensing system is label-free and suitable for the direct detection of antibodies against SARS-CoV-2 in real patient serum samples after coronavirus disease 2019 and/or vaccination.

https://doi.org/10.1016/j.scitotenv.2022.160700

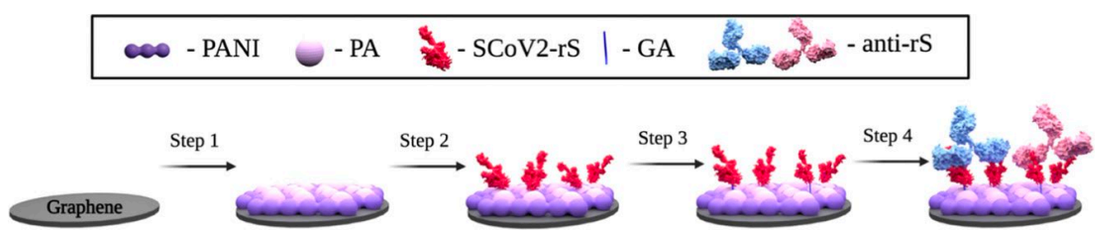

Fig. 6. Scheme of Polyaniline-based electrochemical immunosensor for the determination of antibodies against SARS-CoV-2 spike protein.

Towards molecularly imprinted polypyrrole-based sensor for the detection of methylene blue

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We developed molecularly imprinted polymer-based sensor for methylene blue detection. The sensor was designed by molecular imprinting of polypyrrole with phenothiazine derivative methylene blue (MB) as a template molecule. The molecularly imprinted polymer (MIP) was deposited directly on the surface of the indium tin oxide-coated glass electrode by potential cycling. Different deposition conditions, durability of the layer, and thickness impact were analyzed. The working electrodes were coated with molecularly imprinted and non-imprinted polymer layers. Potential pulse chronoamperometry and cyclic voltammetry were used to study these layers. Scanning electron microscopy was used to determine the surface morphology of the polymer layers. The change in optical absorption was used as an analytical tool to evaluate the capability of the MIP layer to adsorb MB. Selectivity was monitored by tracking the optical absorption changes in the presence of Azure A. In the case of MB adsorption, linearity was observed at all evaluated calibration plots in the concentration range from 0.1 µM to 10 mM. The novelty is in a methodology of the fabrication process of the sensors for MB, where MB retains its native (non-polymerized) form during the deposition of the MIP composite.

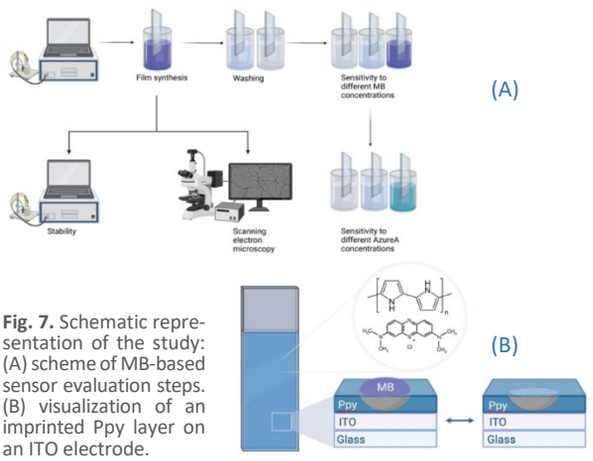

Fig. 7. Schematic representation of the study: (A) scheme of MB-based sensor evaluation steps. (B) visualization of an imprinted Ppy layer on an ITO electrode.

https://doi.org/10.3390/chemosensors11110549

Investigation of BiVO4-based advanced oxidation system for decomposition of organic compounds and production of reactive sulfate species

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Growth of population and expansion of industries lead to increasing contamination of the environment with various organic pollutants. If not properly cleaned, wastewater contaminates freshwater resources and the aquatic environment and has a huge negative impact on ecosystems, the quality of drinking water, and human health. Therefore new and effective purification systems are in demand. In this study, a bismuth vanadate-based advanced oxidation system (AOS) for the decomposition of organic compounds and production of reactive sulfate species (RSS) was investigated. All studied coatings demonstrated high stability in long-lasting photoelectrolysis.

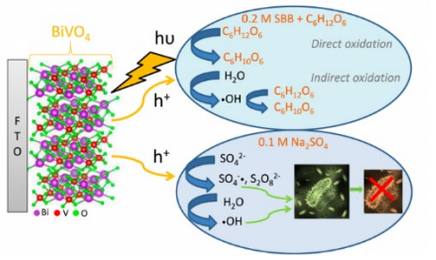

Fig. 8. Scheme of investigation of $BiVO_4$-based advanced oxidation system for decomposition of organic compounds and production of reactive sulfate species.

In addition, the effective light-assisted bactericidal performance of the films in the deactivation of Gram-positive *Bacillus* sp. bacteria was demonstrated. Designed advanced oxidation systems can be applied in sustainable and environmentally friendly water purification systems.

https://doi.org/10.1016/j.scitotenv.2023.162574

Evaluation of the interaction between SARS-CoV-2 spike glycoproteins and molecularly imprinted polypyrrole

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The SARS-CoV-2 spike glycoprotein (SARS-CoV-2-S) was used as a template molecule and polypyrrole (Ppy) was applied as an electro-generated conducting polymer, which acted as a matrix for the formation of molecular imprints. Two types of Ppy-layers, molecularly imprinted polypyrrole (MIP-Ppy) and non-imprinted polypyrrole (NIP-Ppy), were electrochemically deposited on the working platinum electrode. The performance of electrodes modified by MIP-Ppy and NIP-Ppy layers was evaluated by pulsed amperometric detection (PAD), and the integrated Cottrell equation (Anson plot) was used to calculate the amount of charge passed through MIP-Ppy and NIP-Ppy layers. The interaction between SARS-CoV-2 spike glycoproteins and MIP-Ppy was assessed by the Anson plot-based calculations. We found that SARS-CoV-2-S glycoproteins are interacting with MIP-Ppy more strongly than with NIP-Ppy.

https://doi.org/10.1016/j.talanta.2022.123981

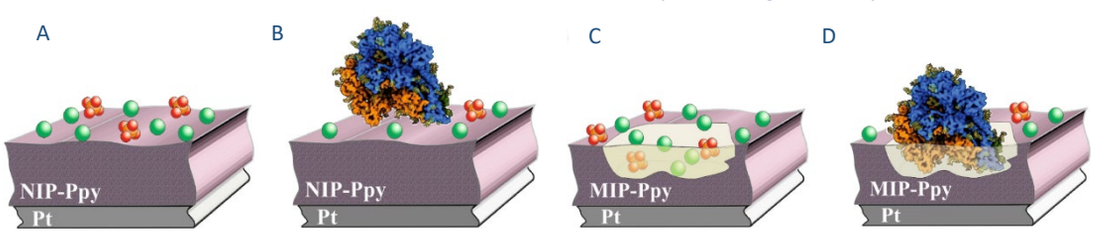

Fig. 9. Interaction of NIP-Ppy and MIP-Ppy with SARS-CoV-2 spike glycoprotein and anions (PO_4^{3-}, HPO_4^{2-} or H_2PO^{4-} and Cl^-). (A) NIP-Ppy and (C) MIP-Ppy in an electrolyte; (B) NIP-Ppy and (D) MIP-Ppy in an electrolyte containing >0 µg/mL of SARS-CoV-2 spike glycoprotein.

The lattice of different magnetizations obtained studying thin polycrystalline manganite film by the modified Ising model. Green and black domains represent spin-up and spin-down domains.

Department of Functional Materials and Electronics

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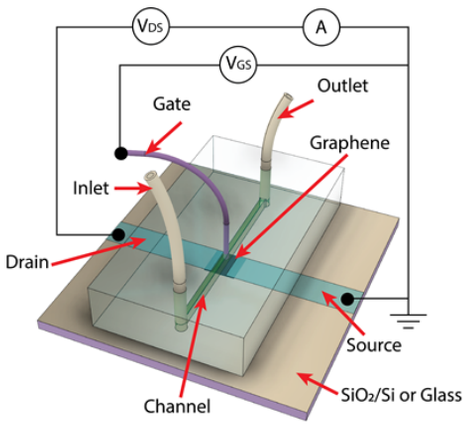
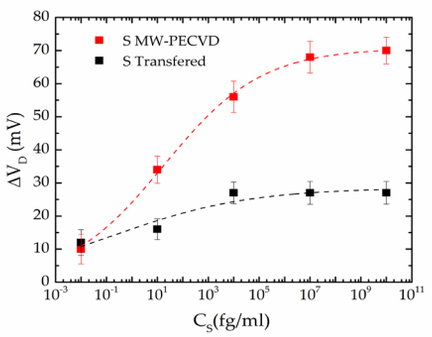
The escalating need for innovative functional materials demonstrating distinct properties in diverse applications is driving the advancement of fabrication technologies in our field. Within the Department of Functional Materials and Electronics, the efforts are underway to develop fabrication technologies, such as pulsed injection MOCVD, magnetron sputtering, and pulsed laser deposition, in order to create advanced thin films and nanostructures. These materials comprise ferromagnetic oxides, Heusler alloys, high-temperature superconductors and 2D semiconductors such as graphene. The fabricated compounds are tailored with specific properties to be used in various applications (spin valves, magnetic field sensors, biosensors, high current limiters and more). Moreover, the numerical calculations as well as experimental investigations of prepared structures and biological cells are performed using various computational tools and experimental techniques. The responses of prepared materials and nanostructures to external stimuli (electrical, magnetic, light, microwaves, etc.) are also studied in our Department. Simultaneously, our research initiatives aim to understand the impact of electrical pulses on plasma membrane permeability across a spectrum of cells, including bacteria, yeast, algae, and mammalian cells. This exploration involves studying how plasma membrane permeability influences the survival of microorganisms equipped with cell walls while identifying specialized testing methodologies. Additionally, we develop and implement the electroporation-based technologies to manage harmful microorganisms. Our investigation extends to analysis of effects of short nanosecond electrical pulses on intracellular signals. Concurrently, efforts are focused on studying the influence of abiotic factors - like light, temperature, and electric fields - on cellular signals. This involves the application of innovative optically transparent polymeric materials for photodynamic therapy and the development of organ-on-a-chip devices to explore electrically induced intercellular signals.

Biosensor based on graphene for detection of COVID-19 Spike S Protein and its entry receptor ACE2

Biosensors based on graphene field-effect transistors (G-FET) for detecting COVID-19 spike S protein and its receptor ACE2 were developed. The graphene, directly synthesized on SiO_2/Si substrate by microwave plasma-enhanced chemical vapor



Graphene biosensor with microfluidic system and measurement scheme.



Change of Dirac voltage ΔV_D vs spike S protein concentrations for MW-PECVD and transferred graphene biosensors.

deposition (MW-PECVD), was used for FET biosensor fabrication. The commercial graphene, CVD-grown on a copper substrate and subsequently transferred onto a glass substrate, was applied for comparison purposes. Graphene surfaces were functionalized by the aromatic molecule PBASE (1-pyrenebutanoic acid succinimidyl ester), and subsequent immobilization of the receptor angiotensin-converting enzyme 2 (ACE2) was performed. A microfluidic system was developed, and transfer curves of liquid-gated FET were measured after each graphene surface modification procedure by varying ACE2 and Spike S protein concentrations. It was demonstrated that the change of the Dirac voltage (ΔV_D) (charge neutrality point) in G-FET transfer characteristics (drain-source current I_{DS} vs gate voltage V_{GS}) was an appropriate parameter for the detection of variations in spike S protein concentration. The testing of the fabricated biosensors shows that the limit of detection (LoD) of this spike protein is as low as 10 ag/mL. The results indicate that transferred as well as MW-PECVD-synthesized graphene-based biosensors demonstrating high sensitivity and low LoD have excellent potential for applications in COVID-19 diagnostics.

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Recognized as an *Editor's Choice Paper*

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Engineering of advanced materials for high magnetic field sensing

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Advanced scientific and industrial equipment requires magnetic field sensors with decreased dimensions while keeping high sensitivity in a wide range of magnetic fields and temperatures. However, there is a lack of commercial sensors for measurements of high magnetic fields B ranging from ~1 T up to megagauss. Therefore, the search for advanced materials and the engineering of nanostructures exhibiting extraordinary properties or new phenomena for high magnetic field sensing applications is of a great importance. The investigations of thin films, nanostructures and two-dimensional (2D) materials, exhibiting non-saturating magnetoresistance (MR) up to high magnetic fields, were reviewed. Tuning of the nanostructure and chemical composition of thin polycrystalline ferromagnetic oxide films (manganites) was shown to lead to a remarkable colossal MR up to megagauss fields. Moreover, the possibility to increase the range of linear magnetoresistive response up to very strong magnetic fields (> 50 T) and large range of temperatures was demonstrated by introducing some structural disorder in different classes of materials, such as non-stoichiometric silver chalcogenides, narrow band gap semiconductors and 2D materials (graphene and transition metal dichalcogenides). The approaches for tailoring the magnetoresistive properties of these nanostructures for high magnetic field sensor applications were discussed and future perspectives outlined.

https://doi.org/10.3390/s23125365

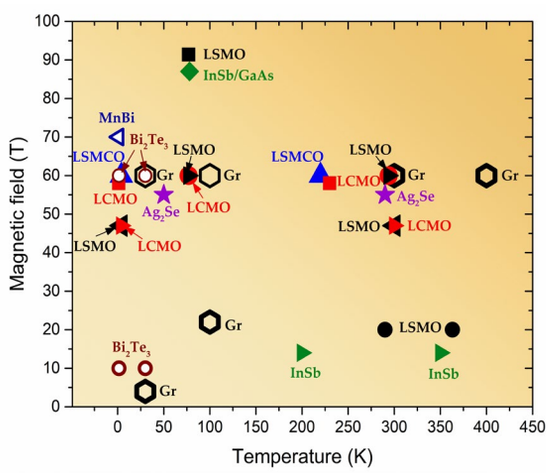

Fig. 1. The ranges of magnetic field and temperature where some classes of magnetic and non-magnetic magnetoresistive materials could be used for development of high magnetic field sensors. Data are taken from different literature sources. The same symbol, but with thinner borders, indicates that quantum oscillations superimposed on MR vs B dependence were observed in high fields at low temperatures. The symbols correspond to La-Sr-Mn-O (LSMO): ●, ◀, ■, ▶; La-Ca-Mn-O (LCMO): ▶ ● ■; La-Sr-Mn-Co-O (LSMCO): ▲; InSb ◆, ▶; Ag_2Se ★; MnBi ◁; Bi_2Te_3 ○○; graphene (Gr) ⬡⬡.

LSMO films grown on Si/SiO_2 substrate for magnetic field sensors applications

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The magnetoresistance (MR) and resistance relaxation of nanostructured $La_{1-x}Sr_xMn_yO_3$ (LSMO) films with different film thicknesses (60–480 nm) grown on Si/SiO_2 substrate by a pulsed-injection MOCVD technique were measured and compared with the reference manganite $LSMO/Al_2O_3$ films of the same thickness. It was found that the high-field MR values were comparable for all investigated films (−40% at 10 T), whereas the memory effects differed depending on the film thickness and substrate used for the deposition. It was demonstrated that resistance relaxation to the initial state after removal of the magnetic field occurred in two time scales: fast (~300 μs) and slow (longer than 10 ms). The testing of the $LSMO/SiO_2/Si$-based magnetic sensors in an alternating magnetic field with a half-period of 22 μs demonstrated that these films could be used for the development of fast magnetic sensors operating at room temperature. For operation at cryogenic temperature, the $LSMO/SiO_2/Si$ films could be employed for single-pulse measurements only due to magnetic-memory effects.

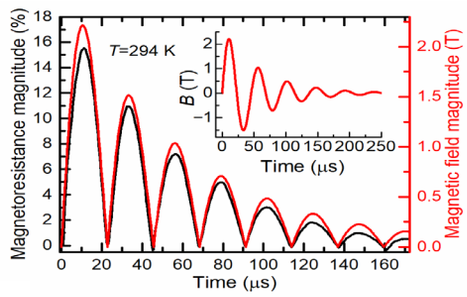

Fig. 2. Testing of magnetic field sensor based on $LSMO/SiO_2/Si$ film: MR dynamics (black curve) of 160 nm-thick film when an alternative magnetic field with damping amplitude (see inset) was applied. Red curve represents magnetic field waveform measured using the LSMO sensor.

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Application of PEF processing to alter the structure of casein proteins

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Caseins represent approximately 80% of the total protein content in milk. Due to their nutritional and functional properties, caseins can be applied as an intermediate compound for pharmaceutical industries. They are also used in many food applications such as nutritional supplements, thickeners, emulsifiers and texture stabilizers. Based on previous studies, alternating structures of proteins can improve their emulsifying and gelling characteristics. Here, pulsed electric field (PEF, 0-30 kV/cm) was applied to study its effects on the physicochemical and structural properties of micellar casein (CSMs). PEF treatment leads to changes in the surface hydrophobicity and protein solubility. The examination of the Amide I region indicated that applying PEF to CSMs decreased the α-helix levels while boosting the β-sheet content. The results of Raman spectroscopy demonstrate that PEF treatment with fields exceeding 10 kV/cm enclosed tyrosine (Tyr) residues within a hydrophobic setting. Moreover, the primary impact of PEF treatment affects the alterations in disulphide linkages. In conclusion, PEF can be employed as an eco-friendly technology to change the structure, physiochemical and techno-functional properties of CSMs.

https://doi.org/10.3390/polym15153311

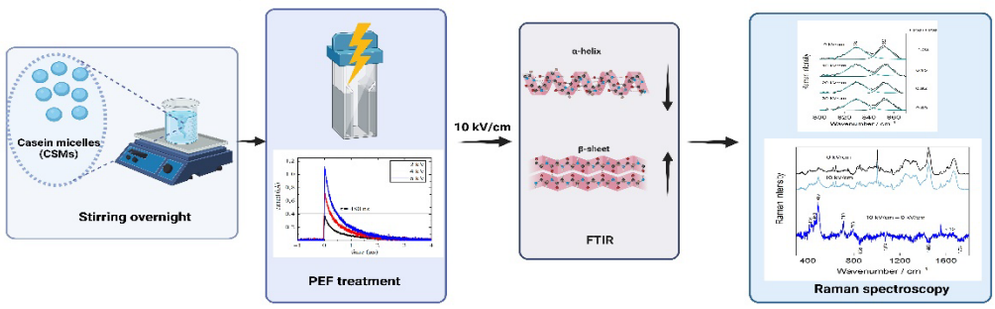

Fig. 3. Schematic diagram of PEF processing and investigation of physicochemical and structural properties of CSMs

Modeling of monomers, dimers and polymers of deposited Br_2I_2Py molecules

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We simulate the ordering of 1,6-dibromo-3,8-diiodopyrene (Br_2I_2Py) molecules on Au(111) surface. The model employs three (intact, singly and doubly deiodinated) types of Br_2I_2Py molecules. It mimics the situation when majority of intact molecules self-organize into ordered two-dimensional network, while most of doubly deiodinated molecules assemble into long organometallic polymeric rows. We use DFT calculations to determine the values of intermolecular interactions and estimate the organometallic interaction with Au atoms. In Monte Carlo calculations, we obtain the monomeric structure of intact molecules, the dimeric structure of singly deiodinated molecules and the polymeric row structure of (mostly) doubly deiodinated molecules. We observe the coexistence of the monomeric phase (intact Br_2I_2Py) and organometallic dimers, as well as their separation. In mixtures of singly and doubly deiodinated molecules, the dimer rows can be either incorporated into two-dimensional pattern of polymeric chains or separated into their own dimeric structure.

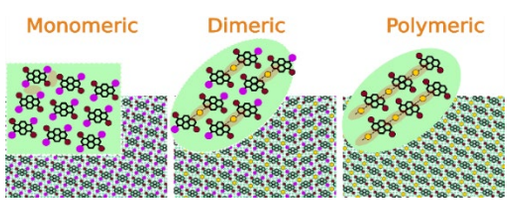

Fig. 4. Ordering of intact (left), singly (middle) and doubly (right) deiodinated Br_2I_2Py molecules at correspondingly room and higher temperatures. Color denotations: I – magenta, Br – brown, Au – yellow and Py – black.

https://doi.org/10.1039/D2CP05463A

Development of a disposable polyacrylamide hydrogel-based semipermeable membrane for micro Ag/AgCl reference electrode

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Currently, most electrochemical biosensors and bioelectrochemical devices use Ag/AgCl-based reference electrodes. However, these standard reference electrodes are large and may not fit in electrochemical cells designed for analysing small sample volumes. It is crucial to develop new designs and improvements for reference electrodes to advance the field of electrochemical biosensors and other bioelectrochemical devices. We created disposable, easily scalable and reproducible membranes suitable for reference electrode design. We have developed castable semipermeable membranes that demonstrate optimal porosity and Cl−ion diffusion. The designed reference electrode was tested in a three-electrode flow system and demonstrated its advantage over commercial

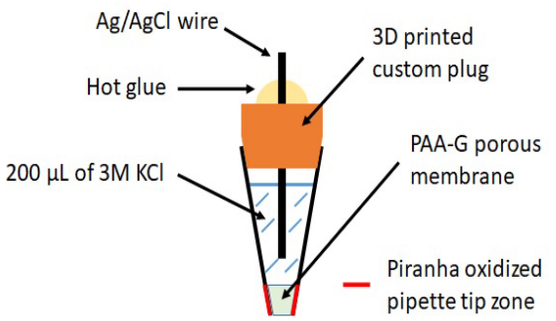

Fig. 5. Schematic drawing representing the design of Ag/AgCl-based reference electrode and setup for the permeability tests.

products. The high response rate of the reference electrode makes the polyacrylamide gel junctions a viable alternative for membrane design, particularly in applications that require the use of high-intensity dyes or toxic compounds, necessitating disposable electrodes.

https://doi.org/10.3390/s23052510

Investigation of osmotic shock effect on pulsed electric field treated S. cerevisiae yeast cells

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Opening up of the outer layer of tiny organisms by pulsed electric field (PEF) treatment is called electroporation (EP). Our goal was to find if EP could be enhanced by quickly changing the liquid environment after the PEF treatment. We were studying plasma membrane and cells recovery process after EP taking into account that a cellular pathway (high osmolarity glycerol (HOG) kinase) might be involved. In yeast, this pathway helps the cells to regain their size and water balance under stress from changes in their surroundings. We tested how cancelling of this pathway affected yeast cells reaction to PEF treatment. Our results showed that yeast cells without a functioning HOG

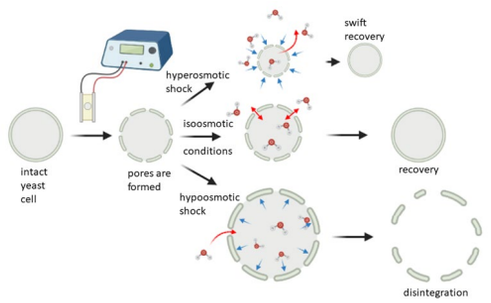


Fig. 6. Schematic representation of post-PEF osmotic shock impact on yeast cell. Blue arrows indicate osmotic pressure on the cell exterior.

pathway were much more sensitive to the electric fields used in the treatment. This confirmed a connection between the HOG pathway and recovery of yeast cells after EP.

https://doi.org/10.1038/s41598-023-37719-4

Scalar Magnetic Field Measuring Probe

EUROPEAN PATENT EP 3893011 B1

The aim of the present invention is to reduce the anisotropy of the magnetoresistance of a scalar magnetic field measuring probe, i.e. to improve the accuracy of measurements when the direction of the magnetic field is not known. A scalar magnetic field measuring probe comprises of three magnetoresistive (MR) sensors (Fig. 7a, 1, 2, 3), each with a respective dielectric substrate coated with a thin film of the material, the electrical resistance of which varies depending on a magnetic field. On the thin film of each MR sensor are locally formed electrically conductive contact areas, to which the wires (4) are attached for connection to electric current source. All three MR sensors

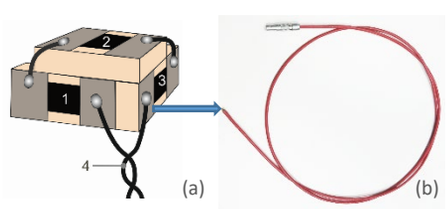


Fig. 7. (a) Scalar magnetic field measuring probe, (b) the probe and the cable.

(1, 2, 3) are arranged in such a way that the plane of the thin film of each of them is perpendicular to the planes of the remaining two sensors. The probe is coated with a sealing filler, wherein the respective conductive contact areas and the connecting wires of three MR sensors (1, 2, 3) are interconnected in such a way that to connect in series thin films of all three MR sensors. A total resistance of a probe is equal to a sum of the resistances of the individual sensors. The material of the thin films is $La_{1-x}[Sr(Ca)]_xMn_{1-y}Co_yO_3$. The electrical resistance of this film depends on magnetic field. The proposed magnetic field probe makes it possible to reduce the anisotropy of the magnetoresistance and maximum measurement error by about 7.9 times (curve 2 in Fig. 8) compared to the measure-ment error of one sensor (curve 1 in Fig. 8).

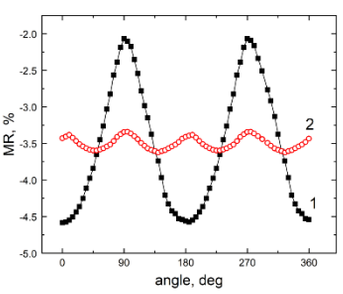
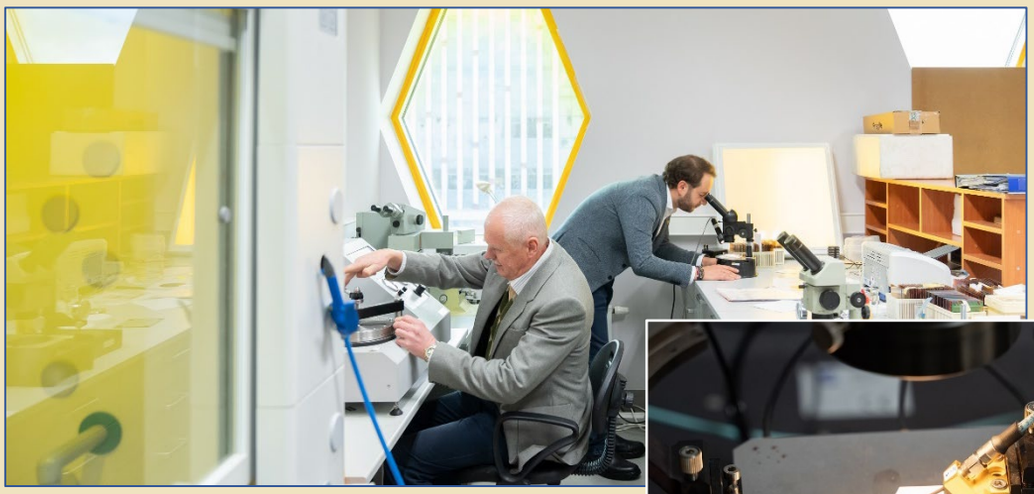
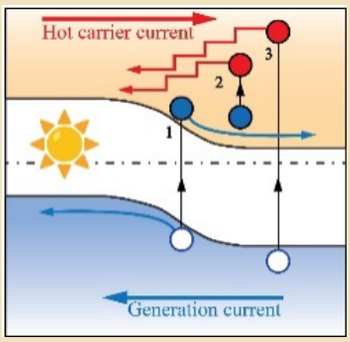


Fig. 8. The dependence of magnetoresistance on the angle between the magnetic field direction and surface of one sensor (curve 1). The same when the probe is composed of three MR sensors (curve 2).





Laboratory of Electronic Processes

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The main activities are focused on:

- investigation of interaction of electromagnetic radiation with semiconductor nanostructures in a wide radiation frequency range;
- investigation of optical transitions in semiconductor nanostructures using single photon counting method;
- solution of Maxwell equations in waveguide systems and metamaterials; development of methods for desynchronization and damping of interacting oscillator arrays; study of carrier dynamics in perovskite and inorganic solar cells; development of innovative devices for microwave, terahertz and quantum electronic applications.

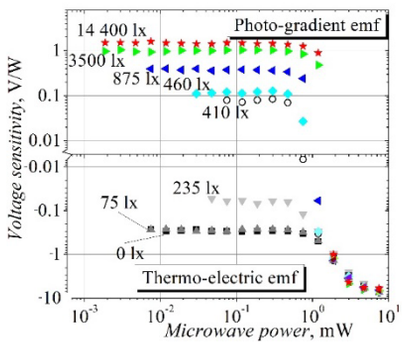

Fig. 1. Dependence of voltage sensitivity of the bow-tie diode on incident microwave power at different white light illuminance values.

Competition between direct detection mechanisms in planar bow-tie microwave diodes on the base of InAlAs/InGaAs/InAlAs heterostructures

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Our study of the voltage–power characteristics, the voltage sensitivity dependence on frequency in the Ka frequency range, the dependence of detected voltage on temperature and its relaxation characteristics in the selectively doped InAlAs/InGaAs bow-tie-shaped semiconductor structures allows to conclude that photo-gradient electromotive force arises the in bow-tie diodes under simultaneous microwave radiation and light illumination.

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Study of ellipsoidal nanowire metamaterials for biomedical applications

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We study the effective properties of surface waves at the boundary of ellipsoidal nanowire metamaterial. Our model could possibly be applied in a clinical practice of cancer detection, since it demonstrates some similarities with real biological systems containing cancer cells as ellipsoidal inclusions.

https://doi.org/10.1007/s11082-023-05369-5

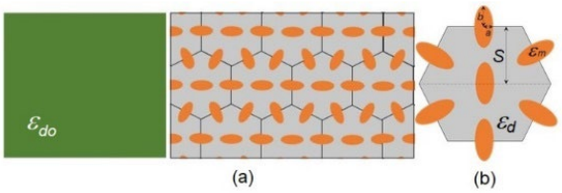
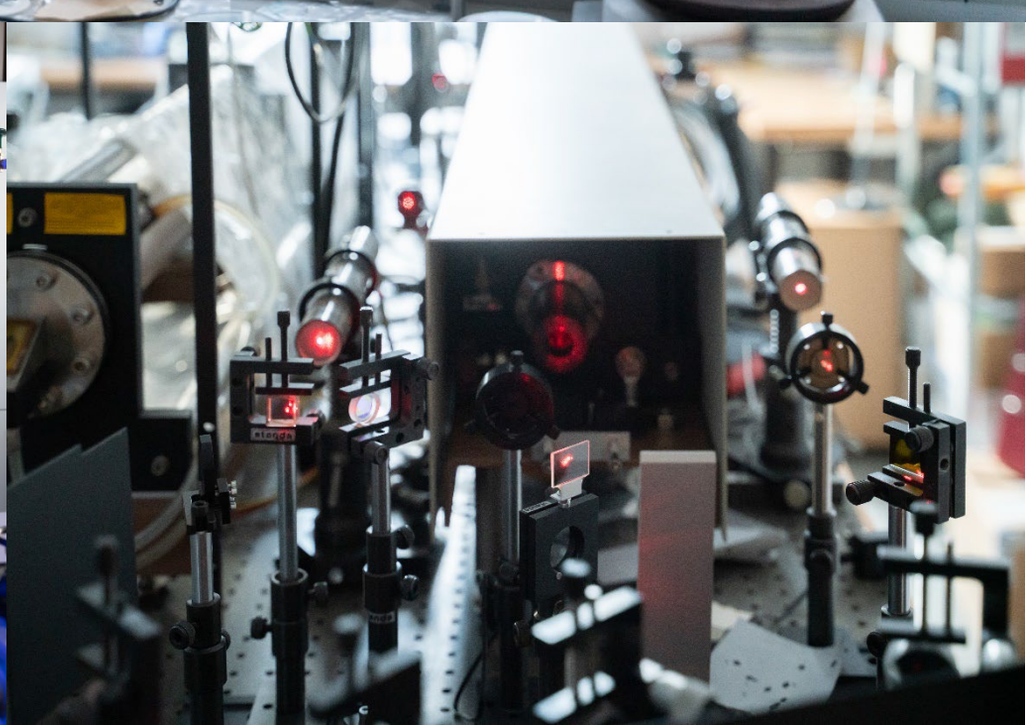
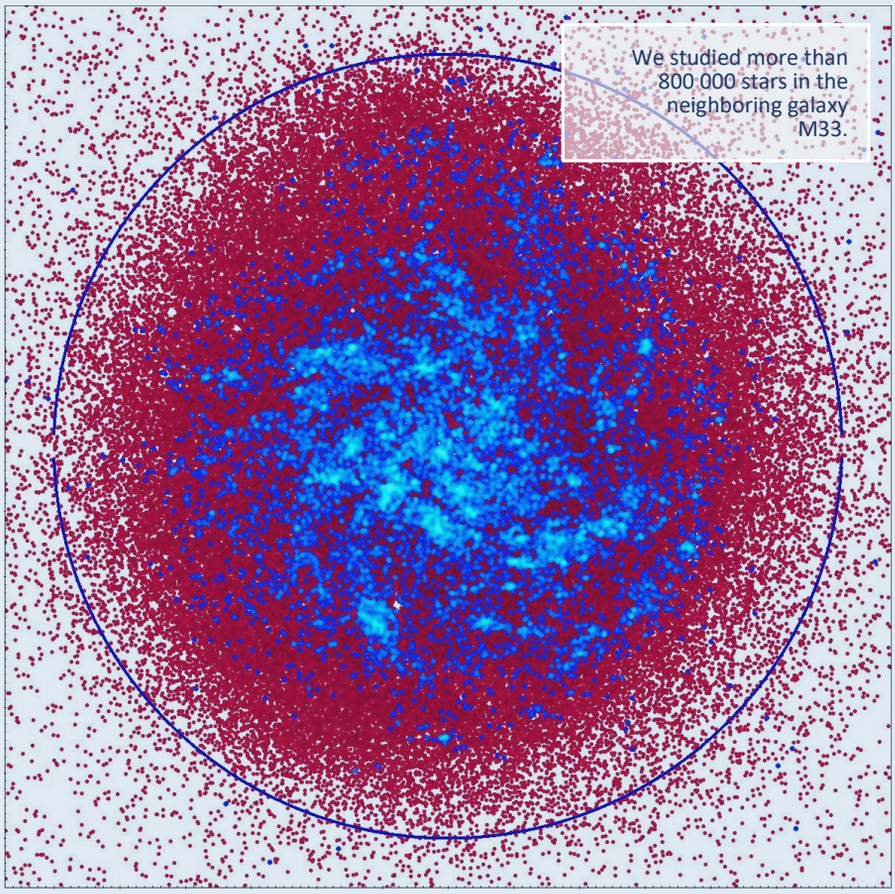


Fig. 2. A schematic representation of (a) ellipsoidal metamaterial boundary and (b) unit cell of metamaterial.

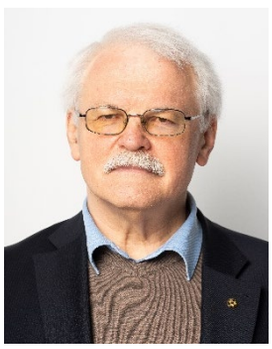




Department of Fundamental Research

The main goal of the department is to create high-level scientific knowledge for increasing competitiveness of the country in the long-term perspective. Research directions are aimed at developing and improving theoretical and experimental methods for solving fundamental problems of biophysics, solid state physics, optics, and astrophysics. The current tasks of the department:

- Application of nonlinear dynamics and control theory methods to the study of complex neural network systems.
- Development and application of electronic structure theory methods for the study of optoelectronic phenomena in semiconductors.
- Development and application of fluctuation methods for the study of wide-bandgap semiconductors.
- Engineering of vector optical fields: generation and study of behavior in photonic systems.
- Studying the evolution of megasystems using artificial intelligence methods.



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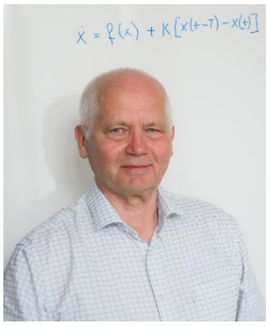
Effect of Cauchy noise on a network of quadratic integrate-and-fire neurons with non-Cauchy heterogeneities

We analyze the dynamics of large networks of pulse-coupled quadratic integrate-and-fire (QIF) neurons driven by Cauchy noise and non-Cauchy heterogeneous inputs. Two types of heterogeneities defined by families of q-Gaussian and flat distributions are considered. Both families are parametrized by a positive integer n, so that for n=1 the distributions in both families coincide with the Cauchy distribution, but as n increases to infinity, the first family tends



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to a normal distribution, and the second to a uniform distribution. For both families, exact systems of mean-field equations are derived and their bifurcation analysis is carried out. In contrast to previous publications, we show that noise and heterogeneity can have qualitatively different effects on the collective dynamics of neurons. Remarkably, changes in noise and heterogeneity in opposite directions can lead to the same bifurcation at the macroscopic level. In particular, collective limit cycle oscillations can be induced by either a reduction in noise or an increase in quenched heterogeneity. An example of a qualitative similar macroscopic effect caused by a decrease in noise or an increase in quenched heterogeneity is shown in Figure. Panels (a) and (b) show, respectively, the dynamics of the mean firing rate and raster plots of the QIF network at a sufficiently high noise intensity and a small value of the heterogeneity parameter. Here, the mean firing rate is almost constant, and the raster plots show the incoherent spiking of neurons over time. Panels (c) and (d) show what happens when the noise intensity decreases for a fixed value of the heterogeneity parameter. The network now exhibits coherent synchronized oscillations. Finally, panels (e) and (f) show similar coherent oscillations that occur with increasing heterogeneity parameter at a fixed noise intensity.

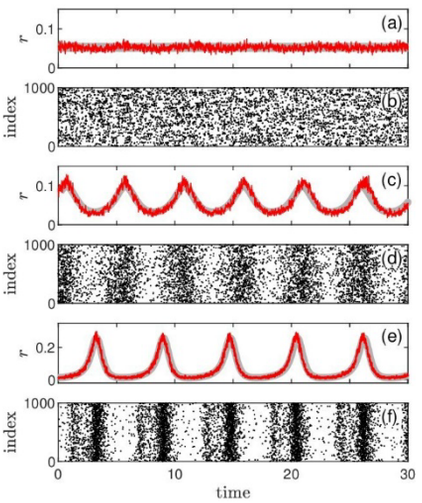

Figure. Dynamics of a population of normally distributed $5{\cdot}10^4$ QIF neurons driven by Cauchy noise and its comparison with the solutions of mean-field equations. Thin red curves represent the solutions of the microscopic model with normally distributed heterogeneity, and thick gray curves are the solutions of mean-field equations. Dots show the spike moments for each neuron, where the vertical axis indicates neuron numbers

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Life after AGN switch off: evolution and properties of fossil galactic outflows

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Active galactic nuclei (AGN) drive massive large-scale outflows of gas in their host galaxies. Once the AGN episode ends, the outflowing gas still has a lot of inertia and can keep expanding for a while. We simulated the evolution of AGN-driven outflows after the AGN switches off in a number of somewhat idealised scenarios. We determined that there is a threshold AGN luminosity, dependent on gas density in the galaxy, necessary for the outflows to persist after the AGN switched off. We also found that fossil outflows detach from the nucleus and become lopsided compared to their driven counterparts. They should be somewhat more common than driven outflows; we suggest that targeted campaigns searching for fossil outflows in inactive galaxies should be undertaken.

https://doi.org/10.1093/mnras/stad1661

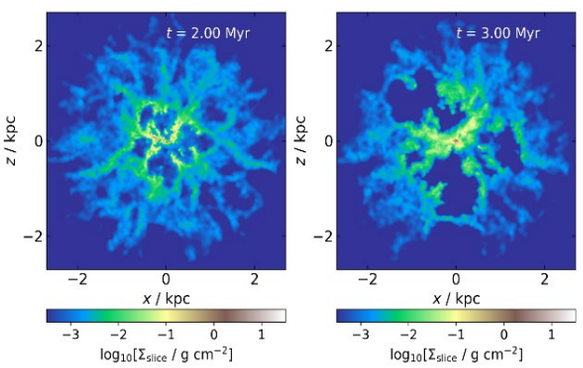

Fig. 1. Evolution of a fossil outflow in a hydrodynamic simulation. Left: gas density at the moment the AGN switches off; the outflow consists of four low-density bubbles. Right: the same simulation 1 Myr later; two of the outflow bubbles have more than doubled in size and detached from the nucleus as they decelerate.

Deriving physical parameter of unresolved star clusters. VII. Adaptive aperture photometry of the M31 PHAT star clusters

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This study is the seventh of a series that investigates degeneracy and stochasticity problems encountered in the determination of age, mass, extinction, and metallicity of partially resolved or unresolved star clusters in external galaxies when using *Hubble Space Telescope* broadband photometry. We present the second part of the global star cluster aperture photometry catalogue for a sample of 1477 star clusters from the M31 PHAT survey.

https://doi.org/10.1051/0004-6361/202347140

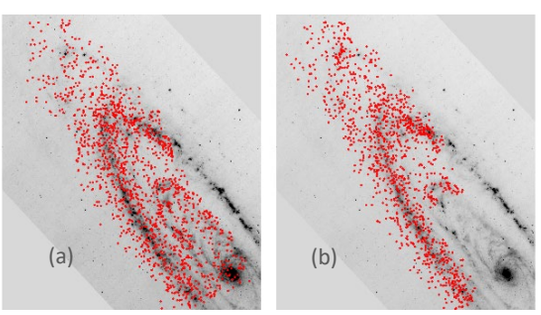

Fig. 2. Locations of measured star clusters on the M31 Spitzer 70 μm map: (a) 1477 clusters measured in this paper; (b) 1181 clusters from Paper VI.

The application of the SCAN density functional to color centers in diamond

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This research evaluates the Strongly Constrained and Appropriately Normed (SCAN) family of meta-GGA density theory functionals for analyzing deep-level color centers in diamonds, specifically nitrogen-, silicon-, germanium-, and tin-vacancies. Traditional methods, like the generalized gradient approximation (GGA), often lack precision in describing the electronic structures of these centers. SCAN and its derivatives, rSCAN and r2SCAN, significantly improve the prediction of optical transition energies, nearly matching the accuracy of computationally demanding hybrid functionals. SCAN enhances the description of potential energy surfaces and luminescence line shapes for the NV- center, outperforming GGA and hybrid methods. Therefore, SCAN functionals are recommended as effective alternatives for the color center studies of solids, especially for computationally demanding tasks.

https://doi.org/10.1063/5.0154319

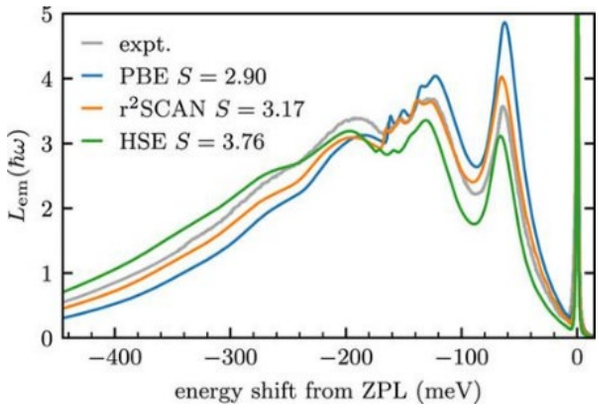

Fig. 3. Theoretical line shapes of normalized NV^- luminescence compared with the experimental spectrum (in eV^{-1}).

Enhancement of spin-to-charge conversion of diamond NV centers at ambient conditions using surface electrodes

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The nitrogen-vacancy (NV) center of a diamond, known for its potential in quantum metrology and computation at ambient conditions, relies on the optical readout of its spin state for various applications. The effectiveness of this process, crucially determined by optical contrast, significantly impacts the NV center's performance. We introduce a high-contrast readout method that employs spin-to-charge conversion with an electrode to modify the NV energy levels, enhancing spin contrast against the conduction band of a diamond. Our theoretical models indicate a potential optical spin contrast of 42% at room temperature, setting a new record for NV centers. This approach also paves the way for diverse new research directions of NV centers, which are explored in our study.

https://doi.org/10.1103/PhysRevB.107.134111

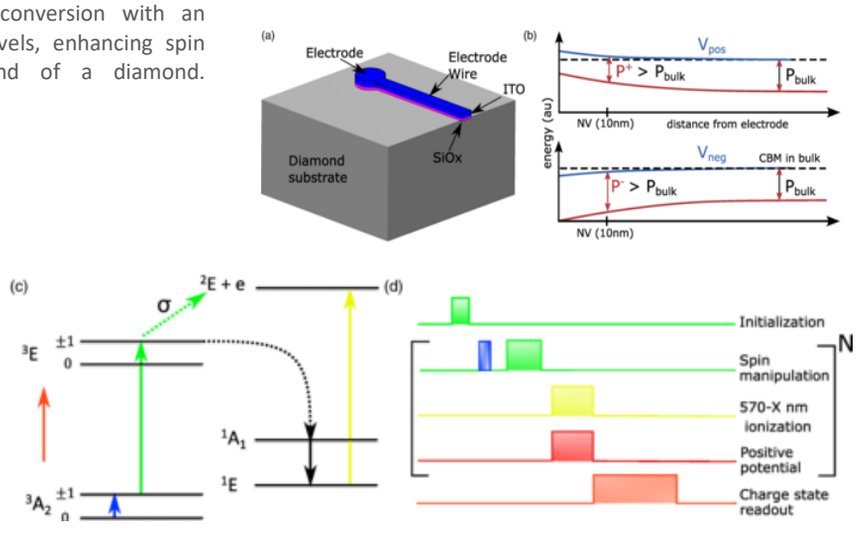

Fig. 4. (a) A cylindrical electrode above a near-surface NV center (10 nm deep) and its connecting wire to a power supply. (b) The electrode's potential affects energy levels: a positive potential raises the conduction band and NV levels, reducing the photoionization energy gap (P+), while a negative potential lowers these levels, increasing the gap (P−) compared to bulk diamond. (c) Energy diagram of the spin-to-charge conversion (SCC) protocol. (d) Pulse sequence for the SCC protocol, showing electrode pulsing during ionization.

Hot-electron drift velocity in (Be)ZnMgO/ZnO 2DEG channels

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We present experimental study of hot-electron transport in ZnO/ZnMgO and BeZnMgO/ZnO heterostructures, containing two-dimensional electron gas (2DEG) channels of two polarities with electrons accelerated by a pulsed electric field. The measurements using electrical pulses of 2-10 ns in duration ensure the control of a self-heating effect. The hot-electron effect, leading to the deviation from the Ohm's law, is evident at moderate and high (>20 kV/cm) electric fields. The monotonous increase in the electron drift velocity is observed at the electric field ranges limited by self-heating effect, leading to the sample damage or breakdown. A high velocity value of $2.0 \cdot 10^7$ cm/s at 270 kV/cm is attained for the channels with BeZnMgO barrier. A highest values of $1.3 \cdot 10^7$ cm/s at 360 kV/cm and of $2.5 \cdot 10^7$ cm/s at 320 kV/cm are estimated for the channels with ZnMgO barrier and bulk ZnO, respectively. The effect of hot phonons at high electric fields on velocity results is discussed.

https://doi.org/10.1088/1402-4896/aca5cd

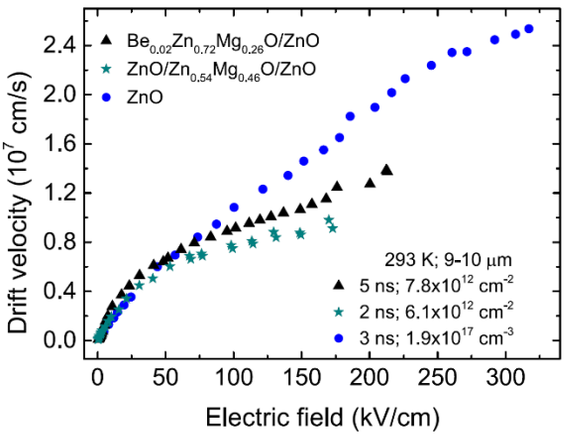

Fig. 5. Electron drift velocity as a function of electric field for $ZnO/Mg_{0.46}Zn_{0.54}O$ (stars), $Be_{0.02}Zn_{0.72}Mg_{0.26}O/ZnO$ 2DEG channels (triangles) and ZnO 3DEG channels (circles) at room temperature. Carrier densities and voltage pulse durations are: $6.1 \cdot 10^{12}$ cm^{-2} and 2 ns (stars), $7.8 \cdot 10^{12}$ cm^{-2} and 5 ns (triangles), and $1.9 \cdot 10^{17}$ cm^{-3} and 3 ns (circles). Sample length is 9 μm (triangles) and 10 μm (stars and circles).

Accelerating Airy beams with particle-like polarization topologies and free-space bimeronic lattices

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Phase and polarization singularities in electromagnetic waves are usually attributed to one-dimensional topologies - lines, knots, and braids. Recently, particle-like structures, such as optical Skyrmions, vortices with spherical polarization, etc., have been predicted and observed. Here we devise vector Airy beams with point-like singularity in the focal plane, thus leading to the presence of a particle-like topology. We present an extensive analytical analysis of the spatial spectra and focal structure of such beams. We report on the presence of a free-space lattice of bimerons in such vector Airy beams.

https://doi.org/10.1364/OL.483339

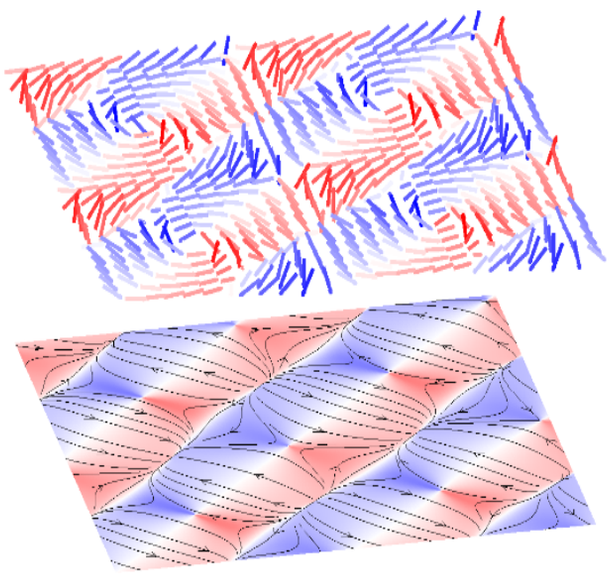

Fig. 6. Distribution of topological charges in the Airy beam.

Department of Environmental Research

The activities of the Department focus on the development and improvement of fundamental principles, technologies, and solutions to reduce risk and exposure to pollution levels by utilizing state-of-the-art tools and methods which are applied to identify the causes and the processes of industry and transport impact on the environmental quality. The department develops and examines:

- Pollution dynamics, transformation, aging processes, physicochemical characterization and source apportionment;
- The formation of aerosol particles, sources, behavior, deposition, control, transport and fate;
- Indoor air quality, exposure and human health;
- Emissions and pollution control technologies;
- Optical properties of aerosol and associated radiative forcing.

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Main achievements:

Involvement in Horizon Europe EDIAQI project which aims to study indoor air pollution (including microplastic) in European cities to understand the sources, routes of exposure, and health effects of indoor air pollution.

The first study aimed to measure airborne nano-sized plastic particles in live human bronchoalveolar lavage fluid samples was conducted. This pioneering research not only uncovered the plastic pollution content in the lower airways of Northern Europe residents but also symbolized significant progress in understanding the biological effects of inhaled microplastic.

LIDAR measurements – unique Lithuanian and Polish scientific project: for the first time a remote sensing study of modifications of aerosol properties was conducted in Vilnius.

New evidence of the presence of micro- and nanoplastic particles in bronchioalveolar lavage samples of clinical trial subjects

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This is the first study reporting the presence of airborne nano-sized plastic particles in the bronchoalveolar lavage fluid (BALF) samples of patients undergoing diagnostic bronchoscopy in the lower airways of the residents of Northern Europe. Human BALF samples were assessed by means of optical and transmission electron microscopy coupled with energy-dispersive X-ray spectroscopy (TEM-EDX). Microplastic particles (MPs) were detected in all BALF samples and ranged from 0.11 ± 0.02 to 12.80 ± 0.64 MPs/100 ml of BALF. Most of the MPs (92.41%) were found in the size range of 10–300 µm.

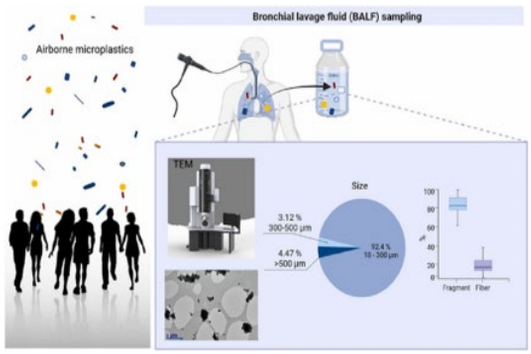

Fig. 1. Schematic diagram of investigated airborne microplastics in bronchoalveolar lavage fluid (BALF) samples of patients.

https://doi.org/10.1016/j.heliyon.2023.e19665

Long term observations of biomass burning aerosol over Warsaw by means of multiwavelength lidar

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High quality lidar measurements of PollyXT operating at the University of Warsaw in 2013-2022 were analyzed to present a comprehensive optical characterization of biomass burning aerosols (BBAs) over Warsaw. BBA layers were identified for a given year by sector of origin. It was shown that as aerosol's age increases, there is more backscattering and less extinction at 355 nm in relation to 532 nm. The analysis of the lidar ratio demonstrated that the main changes of the aging process were observed in the UV spectra.

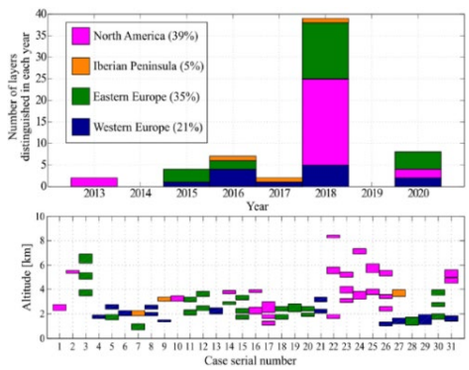

Fig. 2. (Top) Number of the BBA layers identified from lidar measurements in Warsaw in a year, divided into BBA origin sector. (Bottom) Number and height of the layers distinguished on the profiles selected for analysis.

https://doi.org/10.1364/OE.496794

Impact of long-range transport on black carbon source and optical properties of aerosol particles in two urban environments

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We studied the properties of light-absorbing aerosol particles and the impact of long-range transport of air mass on black carbon (BC) in urban environments of Warsaw (Poland) and Vilnius (Lithuania). The BC mass concentration and the aerosol optical properties (scattering Ångström exponent (SAE), absorption Ångström exponent (AAE), and single scattering albedo (SSA)) were analysed. The BC concentration decrease was found similar at both sites (42% in Warsaw and 50% in Vilnius), but the increase was twice higher in Vilnius (64%) than in Warsaw (30%). However, both sites exhibited a comparable abundance (90%) of submicron (SAE<1.3) BC-dominated (AAE<1.5) particles.

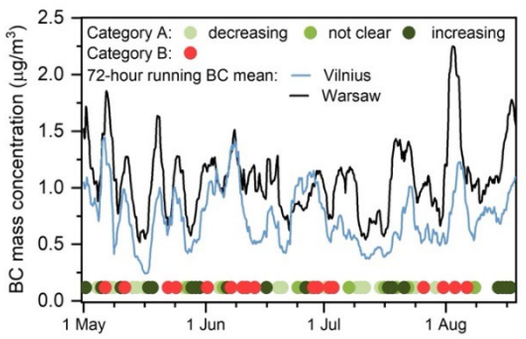

Fig. 3. Time series of 72-h running mean of BC mass concentration in May – August 2022. The circles mark air mass trajectory classification: category A – overlapping trajectories, B – different sources and pathways.

https://doi.org/10.1016/j.heliyon.2023.e19652

Fabrication of chitosan-palladium nanoparticles by liquid atomization

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The aim of this research was to produce chitosan-palladium nanoparticles. The complex was synthesized from chitosan reaction with palladium salt ($PdCl_2$), and nanoparticles were generated using various liquid atomization techniques. The smallest chitosan-palladium nanoparticles (D_g =15±3 nm) were obtained by electrospray method. The chemical characterisation of deposited nanoparticles was performed using coherent anti-Stokes Raman scattering microscopy (CARS) by utilising a chitosan specific vibrational signal of N–H at 3290 cm^{-1}.

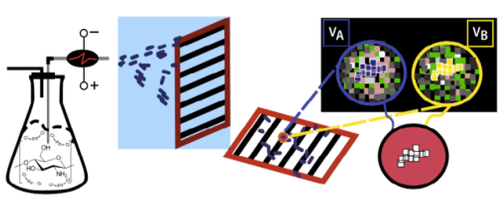

Fig. 4. The illustrative diagram of a setup for chitosan-palladium nanoparticle production by liquid atomization and electrospray techniques, following chemical characterisation of chitosan species using CARS.

https://doi.org/10.1007/s10924-022-02665-1

Long-term spatial and temporal evaluation of the $PM_{2.5}$ and PM_{10} mass concentrations in Lithuania

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The long-term data of particulate matter ($PM_{2.5}$, PM_{10}) mass concentration and ratios in Lithuania over 17 years (2006–2022), were analyzed. It was found that 22.95% of days had a $PM_{2.5}$ concentration that exceeded the EU daily limitation (15 μg m^{-3}), and PM_{10} concentrations exceeded WHO guidelines for 19.94% of days. A negative trend is exhibited for $PM_{2.5}$ and PM_{10} at the high mass concentration and an upward trend at statistically insignificant levels ($p > 0.05$) for low mass concentrations of both PM_{10} and $PM_{2.5}$. The daily average $PM_{2.5}/PM_{10}$ ratios vary within a range of 0.15–0.9. The daily average $PM_{2.5}/PM_{10}$ ratios were slightly higher at the urban background (0.52 ± 0.16) than at traffic sites (0.50 ± 0.14) and rural background (0.45 ± 0.17).

https://doi.org/10.1016/j.apr.2023.101951

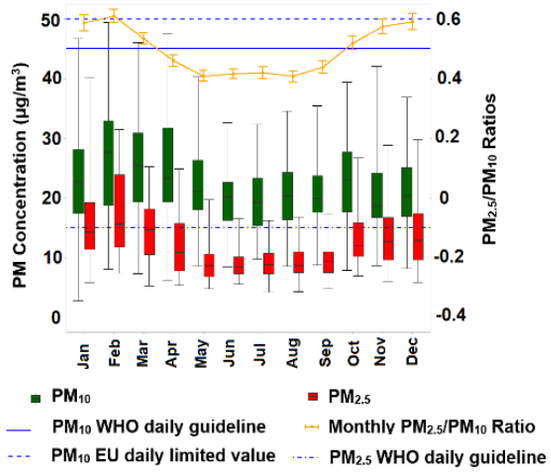

Fig. 5. Monthly variation of the $PM_{2.5}/PM_{10}$ ratios and PM concentrations during the study period.

Effect of graphene oxide on the uptake, translocation and toxicity of metal mixture to garden cress plants: mitigation of metal phytotoxicity due to nanosorption

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This research was focused on examination of the phytotoxicity of different concentrations of graphene oxide (GO) and its co-exposure with the metal mixture (MIX, Ni^{2+}, Zn^{2+}, Cr^{3+} and Cu^{2+}) using garden cress (*Lepidium sativum L.)* as a test organism. In most cases the tested concentrations of MIX, GO and MIX+GO did not affect seed germination, root growth and biomass of roots and seedlings, however, they were found to alter photosynthesis processes, enhance production of carotenoids and H_2O_2, and activate lipid peroxidation.

https://doi.org/10.1016/j.chemosphere.2022.137221

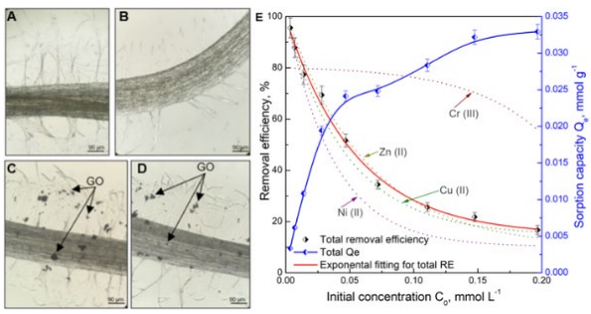
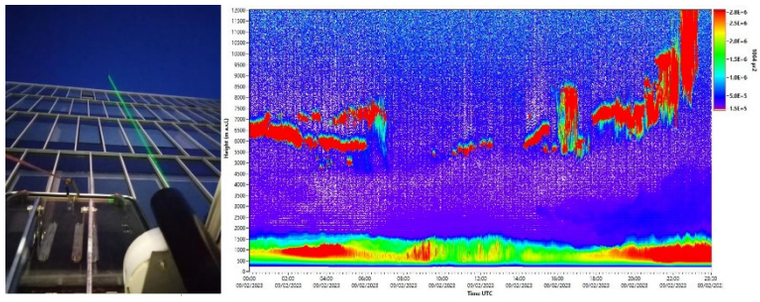


Fig. 6. *Lepidium sativum L.* roots in light microscope images (black arrows show GO distribution) after exposure to (A) control, (B) MIX80, (C) 80 mg/L GO and (D) MIX+GO80. (E) The dependence of GO sorption capacity (Q_e) on the initial concentrations of Cr (III), Cu (II), Ni (II) and Zn (II) in MIX and the comparison of GO efficiency for the removal of each metal and the total amount using the exponential fit.

Importance of long-range transport of BIOmass burning emissions to local Smog events in Urban Environments (BIOSURE)

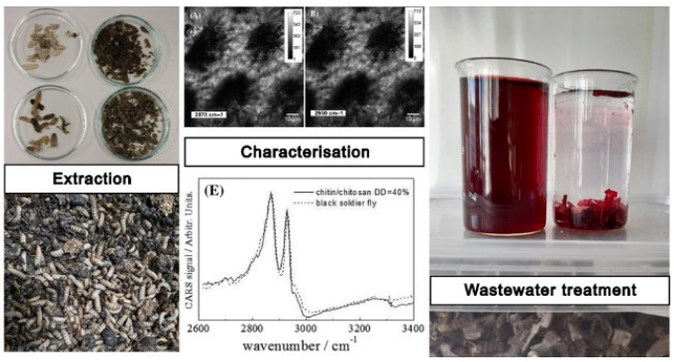
LIDAR measurements – unique Lithuanian and Polish scientific project: for the first time remote sensing study on aerosol properties modifications will be conducted between observational sites.



ESA Mobile Raman lidar (EMORAL) developed by ESA PLIIS programme POLIMOS and 2023.02.09 24-h measurements.

By combining in situ and remote sensing data, the results of this study have provided a unique possibility to separately evaluate the importance of local and long-range transport-related Biomass Burning Aerosol to the air quality in urban environments in Vilnius and Warsaw. It was investigated that during the warm season, biomass burning contributes significantly less to atmospheric composition in Warsaw and Vilnius than fossil fuel combustion.

Bilateral research funding programme between Research Council of Lithuania (LMT) and National Science Centre of Poland (NCN): DAINA-2 Polish-Lithuanian Funding Initiative "Importance of long-range transport of BIO mass burning emissions to local Smog events in Urban Environments (BIOSURE)" under project agreement No. P-LL-21-130.



International R&D project EUREKA E!13636

The researchers team from the Department Environmental Research with partner JSC "REKIN" have successfully completed EUREKA E!13636 research project by utilising black soldier fly (*Hermetia illucens*) from its different life cycle stage for chitin/chitosan-based sorbent production. Fly farming on industrial scale is an innovative and environmentally friendly approach to a food wasting problem. Fly shells from larval and pupal stages are considered as waste, however they are rich in chitin and is a promising source for chitosan production. A new chitosan-based sorbent was produced for the treatment of wastewater contaminated with heavy metals and azo dyes and successfully tested on industrial scale.

International R&D project EUREKA "Use of modified fly (*Hermetia lilucens*) larva shells and dead flies for the wastewater treatment," Nr. 01.2.2-MITA-K-702-12-0008.

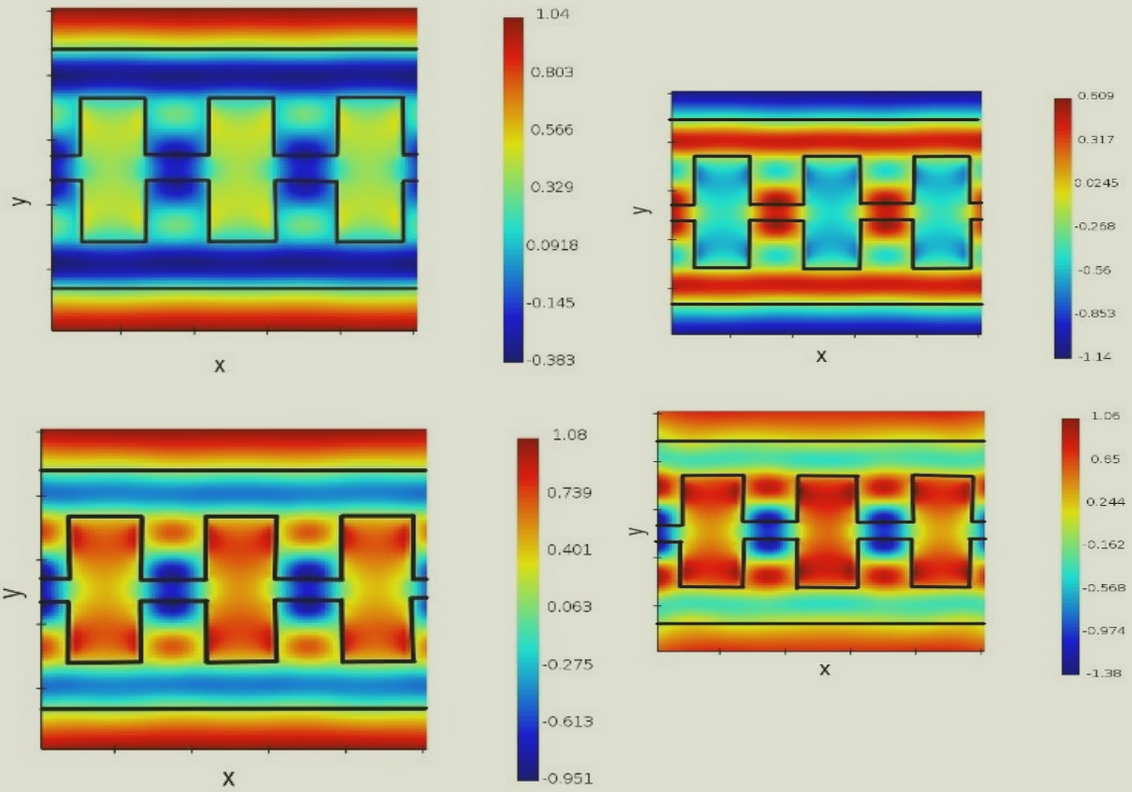
Department of Environment research is participating in HORIZON EUROPE project EDIAQI (Evidence driven indoor air quality improvement)

with 18 leading European organizations which join forces to address and tackle the emerging threats of indoor air pollution and to promote living and working in healthy environments in Europe.

The goal of the project is to validate user-friendly IAQ monitoring solutions, also through a series of pilots and campaigns, that can help create a long-term Europe-wide knowledge base for risk factors associated with standard and novel indoor air pollutants. The evidence provided along with the characterization of main sources of indoor air pollutants for relevant and representative indoor environments will help supporting relevant stakeholders with standardized guidelines for interventions to improve IAQ policy-makers in revising IAQ standards and supporting measures for IAQ regulation, control and monitoring as well providing science-based evidence for supporting the Zero-Pollution Action Plan of the European Green Deal. Key results on machine learning (hybrid digital twin) and model simulations will allow to better understand processes related to indoor-outdoor pollution exchange and transformation. More specifically, the project will characterize sources and routes of exposure and dispersion of chemical, biological, and emerging indoor air pollution in multiple cities in European Union. EDIAQI will also aim to quantify the main properties of pollutants and processes through a dual approach in which the project team will 1) carry out state-of-the-art, small-scale, high-intensity scientific focus measurement campaigns; and 2) investigate the long-term, large-scale monitoring of target indoor air pollutants. The experts from FTMC will contribute above all their competence on aerosol particles, health impact, and exposure to micropollutants including microplastics. The chosen project strategy for developing, characterization, and deployment of cost-effective/user-friendly monitoring solutions, together with the-state-of-the-art scientific instrumentation will allow to create new knowledge on sources, routes of exposure, and body burdens of indoor multipollutant.

Dr. Sebastian Düsing from the Leibniz Institute for Tropospheric Research (TROPOS) came to help the project partners start the measurements campaign.

The EDIAQI project has received funding from the European Union's Horizon Europe framework programme under the Grant Agreement n. 101057497 – call HORIZON-HLTH-2021-ENVHLTH-02.



Department of Nuclear Research

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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. The processes, related to nuclear materials and ionising radiation analysis, focusing on both safety of nuclear installations and new technologies, are studied in the *Experimental Nuclear Research Laboratory*. This includes participation in multinational radioactive waste management projects on radioactive waste predisposal and deep geological disposal management. Development of ion beam methods for material analysis and modification is an important part of our activities having intersections both with semiconductor materials and applications for lasers. We also study organic scintillator films exploring inexpensive materials which might be applied for detection and spectroscopy of ionizing radiation particles. The principles of high energy particle acceleration are investigated using ultrashort laser pulses for practical application in dielectric laser accelerator. Complementary information on material properties (magnetic properties, oxidation and corrosion of iron compounds) is determined by Mössbauer spectroscopy which is combined with the data of vibrating sample magnetometer for better characterization of multiferroics. In the *Isotopic Research Laboratory* the special attention is paid to environmental impact assessment of energy generating facilities, impacts 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 investigated. Application of stable isotope ratio analysis ($\delta^{13}C$, $\delta^{15}N$, $\delta^{18}O$ and $\delta^{34}S$) in environmental, archeological and food samples stimulates new promising technologies. The *Accelerator Mass Spectrometry Laboratory* with ^{14}C measurements ensures activities related to carbon dating and analysis of triple carbon ratio for dedicated samples. Close collaboration of all laboratories leads to development of smart-environmental and environment-safe nuclear fuel cycle technologies and implementation of new analysis methods for public and business needs.

^{14}C analysis in water systems. II. Long-range transport and deposition on the Arctic snowpack of nuclear contaminated particulate matter

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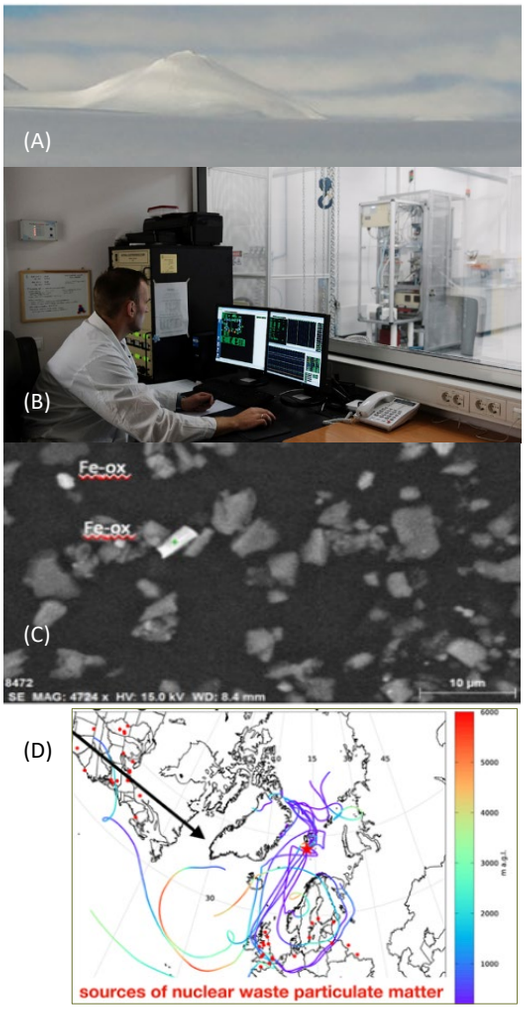
Anomalously high ^{14}C activity has been determined on surface and seasonal snow sampled in early May 2019 on glaciers in the Hornsund fjord area (Svalbard). The high snow concentrations of ^{14}C suggest long-range atmospheric transport of contaminated particles from lower latitudes, possibly from nuclear installations. The analysis of the synoptic and local meteorological data allowed to associate the long-range transport of anomalous ^{14}C concentration to an intrusion event of a warm and humid air mass that likely brought pollutants from Central Europe to the Arctic in late April 2019. Elemental and organic carbon (EC and OC) trace element concentration data and scanning electron microscopy morphological analysis were performed on the same snow samples to better constrain the transport process (see Fig. for detail). In particular, the highest ^{14}C values found in the snowpack (> 200 percent of Modern Carbon, pMC) were associated with the lowest OC/EC ratios (< 4), an indication of an anthropogenic industrial source, and with the presence of spherical particles rich in iron, zirconium and titanium, which suggest an origin related to nuclear waste reprocessing plants. This study highlights the role of long-range transport in exposing Arctic environments to human pollution, given that the frequency and intensity of atmospheric warming events are predicted to increase due to ongoing climate change.

https://doi.org/10.1016/j.jhazmat.2023.131317



Estimated ^{14}C releases from the Ignalina nuclear power plant to Lake Drukšiai.

Optimization of radioactive waste management (RWM) technologies

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Participation in multinational RWM projects (both EU Horizon (EURAD, PREDIS) and other implemented projects) makes it possible to gain and use in practice the newest achievements in RWM technology and knowledge on RW predisposal and deep geological disposal management. The creative adaptation of existing technique -application of $CeBr_3$ measurements with MCNP modeling allows to classify properly the low activity waste and materials with improved effectiveness for in-situ measurement (Fig. 1). The Compton-to-peak ratio of gamma spectra analysis was used for assessment of metallic radioactive waste surface and volume contamination. Inter-comparison of experimental γ-spectra analysis demonstrates that the values of Compton-to-peak ratio depend on the resolutions of detectors: difference between $CeBr_3$ and HPGe detectors varies 4 - 5.6 times. Despite the fact that $CeBr_3$ is characterized by 10 times lower sensitivity it is still suitable for in-situ measurements of metallic radioactive waste for identification of surface and volume contamination (Fig. 2).

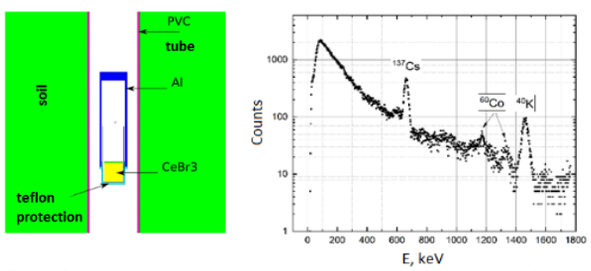

Fig. 1. Schematic diagram of the model of the $CeBr_3$ detector in the borehole and measured spectrum of ^{60}Co and ^{137}Cs in the well (0.13 Bq/g ^{137}Cs activity).

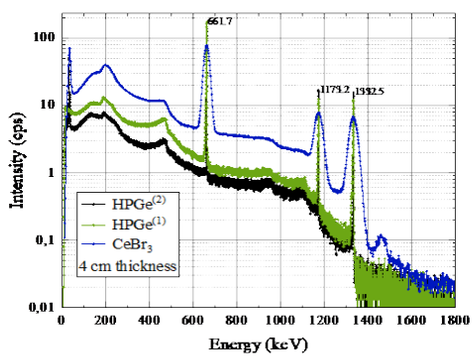

Fig. 2. Comparison of spectra of shielded (4 cm metal screen) ^{60}Co and ^{137}Cs sources using $CeBr_3$ scintillation and two HPGe detectors.

Carbon fluxes from river to sea

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Sources and fate of carbon (C) in a shallow, coastal lagoon have been investigated to understand the global C cycles and sources of organic matter supporting food webs. Lagoons act to transport, retain (via sedimentation) and divert (via outgassing) carbon on its route from land to sea. A carbon budget for a large coastal lagoon in the Baltic region, that incorporates measurements of river-estuary, estuary-marine, and sediment-water exchanges, along with internal processes (production and respiration) governing transformations among C fractions was evaluated. Organic C fluxes were dominated by internal cycling (gross primary production (GPP) and respiration (R)), whereas inorganic C fluxes were largely dependent on hydrological transport. Sediment-water exchange of dissolved inorganic and organic carbon (DIC and DOC, respectively) was of lesser importance, despite the shallowness of the lagoon. On an annual basis, the lagoon was a net source of organic matter (OM) to the Baltic Sea as export of dissolved and particulate fractions exceeded riverine and marine inputs by 37±4%. We combined the mass balance and metabolism results with a consumer energetics approach to align C sources with C flows through the lagoon food web.

https://doi.org/10.1007/s12237-023-01214-w

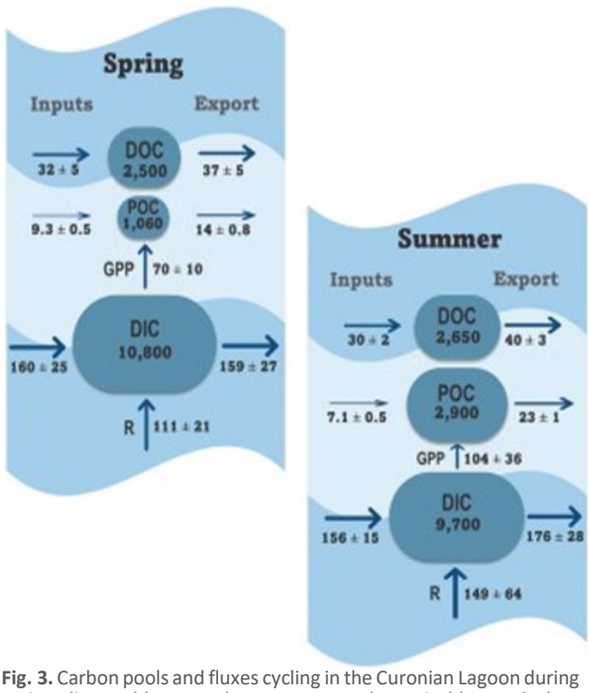

Fig. 3. Carbon pools and fluxes cycling in the Curonian Lagoon during spring diatom bloom and summer cyanobacteria bloom. Carbon pools (boxes) are g C m^{-2}; fluxes (arrows) are g C m^{-2} d^{-1}.

^{14}C analysis in water systems. I. Cooling pond sediments as evidence of nuclear power plant liquid effluents

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In the Case study of Lake Drūkšiai, Ignalina nuclear power plant cooling pond, the vertical distribution of radiocarbon in the three undisturbed bottom sediment cores, taken in 2013 and 2019 within an area of 50-100 m in the deepest depression, were investigated. Typically, radiocarbon distribution studies are not performed on multiple sediment cores from the same lake site, as it is not expected that the carbon cycle at the closely located sites would be affected by different factors. However, our study has shown that both cores taken at the same lake site in 2019 at a distance of 10–20 m from each other can have different 14C distributions in the corresponding layers of the core. The difference was up to 30 pMC (or 0.7 GBq/y), but accounting for the core taken several years ago, the variations reached 1.3 GBq/y. Sediment columns also showed persistent ^{14}C pollution of 0.76□0.06 GBq/y eight years after the closure of the power plan.

https://doi.org/10.1371/journal.pone.0285531

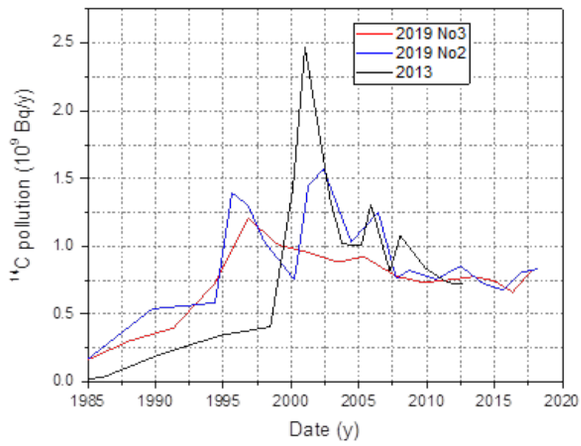

Fig. 4. Estimated ^{14}C releases from the Ignalina nuclear power plant to Lake Drukšiai.

Characterization of particulate matter emissions from internal combustion engines using $\delta^{13}C$ values

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Stable carbon isotope ratio of particulate emissions from internal combustion engines (ICEs) is an important characteristic in atmospheric carbonaceous particulate matter (PM) source studies. Long-term measurements (2009–2020) of $\delta^{13}C$ values of commercial fuels in Lithuania were conducted to evaluate the current isotopic composition of the fuel due to the changing share of renewable energy sources (RES). The experimental results on stable carbon isotope ratio ($\delta^{13}C$) in PM10 emitted by different types of ICEs (two-stroke and four-stroke) were analysed using different driving scenarios on a test bench (idling, NEDC, different torque, and speed). At idle, the following average $\delta^{13}C$ (PM10) values of different fuel types were determined: –27.80‰ for gasoline, –28.97‰ for diesel, –27.89‰ for biofuel-C3, and –16.95‰ for biofuel-C4 (Fig. 5). Isotopic fractionation during combustion in ICEs depended on fuel type. The magnitude of $\delta^{13}C$ was 3‰ for gasoline, 2‰ for diesel, 1.5‰ for biofuel-C3, and 0.6‰ for biofuel-C4. The $\delta^{13}C$ values of ICEs-generated PM10 were found to be dependent on the amount of bio-based components of the fuel, e. g. such as hydro-treated vegetable oil (HVO). However, insubstantial differences were found between the $\delta^{13}C$ of PM derived from pure diesel and the ethanol/diesel blend (E40). Stable isotope ratio method can be used to investigate the amount of RES in the fuel.

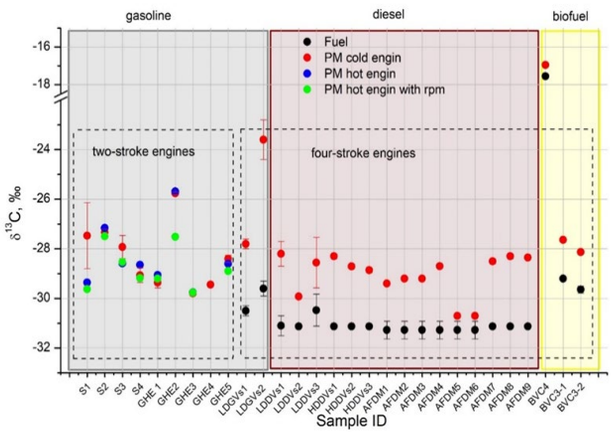

Fig. 5. $\delta^{13}C$ values of initial fuels and PM10 emissions from two-stroke and four-stroke internal combustion engines. On-road transport and non-road mobile machinery were working on idle regimes.

https://doi.org/10.1016/j.apr.2023.101868

Elastic backscattering spectrometry for ion implantation damage

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Elastic backscattering spectrometry (EBS) is a technique for analyzing ion distribution and profiles in samples assessing ion implantation damage and evaluating lattice impurity distribution. By detecting backscattered light particles and analyzing energy spectra, the resonant cross-sections in the complicated experimental geometry are obtained. Crystalline materials introduce additional complexities in spectra due to particle channeling effects, since the particles travel along the strings or planes of atoms. As a result, the energy loss and reaction rates are lower compared to amorphous materials. To address these challenges, a new open-source elastic backscattering spectra simulation tool was developed. Validation of the model was performed using the experimental data for Si, SiC, SiO_2 and diamond samples investigated with 1 – 2.5 MeV energy protons. The results showed a satisfactory agreement of experimental and simulated spectra, particularly as the simulating particle beam spread was maintained below 0.1°. Further analysis at different values of lattice temperature revealed that an increase in temperature heightened backscattering yield, while changes in beam spread significantly altered the spectra. The developed model provides a credible alternative to commercial simulation tools and serves as a solid foundation for channeling EBS simulations.

https://doi.org/10.1016/j.nimb.2023.165091

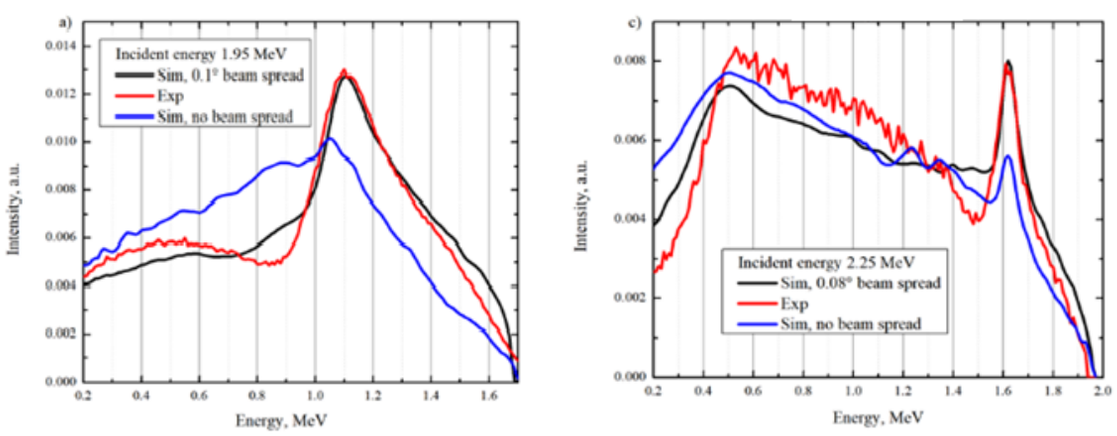
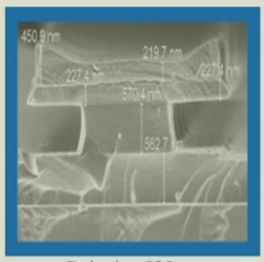
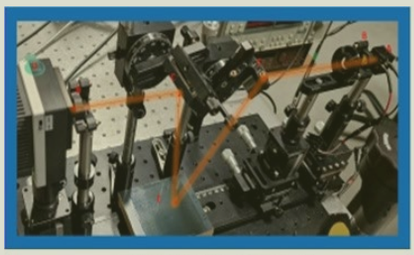


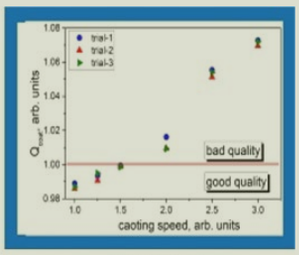
Fig. 6. Experimental and simulated backscattering spectra obtained for protons channel along the <100> axis of Si. Particle energy: (a) 1.95 MeV, (c) 2.25 MeV.



Technology R&D


Device Fabrication


System Design & Integration



Field Testing

Department of Physical Technologies

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Semiconductors for Applied Infrared Photonics. Research of semiconductor characteristics in combination with technology innovation enables us to develop special structures fusing electronic, electrical and optical properties within complex functional elements (left Fig.) Highly attractive ways to make new multi-functional elements emerged from attempts to combine the usual three-dimensional (3D) materials with the two-dimensional (2D) ones. New concepts based on the van der Waals controlled integration principles were proved being highly promising because these structures can change the parameters of multi-functional hybrid system in unexpected ways. Technology studies result in methodically adapted CMOS compatible processes acceptable for fabrication of prototype devices similar to assembled IR lasers shown in the second Fig. Deep understanding of the technology and the device physics allows us to develop high-tech multi-component system combining hybrid and monolithic integration of the elements into it (third Fig.). Meeting the specific needs of the end users, a system platform can be adapted for an on-line non-destructive quality control of products and processes as it was proved by the field tests of the polymer coating control (right Fig.) in the mid-IR laser based project (01.2.2-CPVA-K-703-03-0019). Conversion of the features of processes and things into the output data is the main driving force for the R&D activities on semiconducting nanostructures. Also, highly specific safety and environment related investigations are carried out on microwave interaction with materials, structures and devices.

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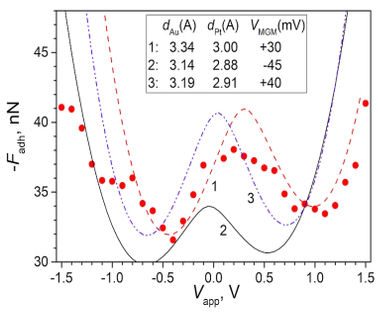
Interface characteristics and external voltage under compressing force in metal–graphene–metal stacks

Metal–graphene–metal (MGM) stacks provide novel way for integration of two-dimensional (2D) materials into three-dimensional (3D) electronic devices. Control of the local electronic properties in the stacks is a primary problem to be solved when developing hybrid structures with 2D and 3D elements. The stack was produced by pressing a Pt probe into the surface of an Au-supported graphene monolayer. The original model was proposed, and the dependences of electrostatic interface forces F_{adh} on applied voltage V_{app} were obtained (see Fig.) which demonstrate the influence of the interface distances, the built-in potential and the overlapping of the states. A route to produce a nano-scale electronic device was also suggested.



Symmetric and asymmetric Fano resonances in a broken axial symmetry metasurface of split ring resonators

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In the metasurface with the broken symmetry of the unit cell consisting of two resonators, two Fano resonances were found instead of one characteristic to the symmetric unit cell. By calculating the phases of currents in the adjacent resonators, it was shown that resonances are different: one is symmetric, while the other one - asymmetric. For symmetric Fano resonance, the currents in the segments of adjacent resonators are parallel to the electric field flow in the same direction, whereas for asymmetric Fano resonance they are opposite. Modelling results were confirmed by experimental investigation of the metasurface spectrum in a microwave frequency range showing two experimentally measured resonances.

https://doi.org/10.1063/5.0167509

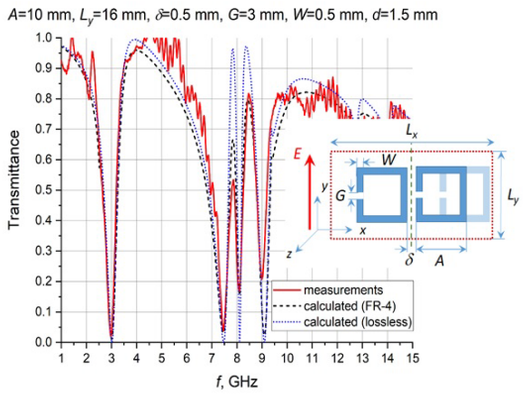

Fig. 1. Measured and calculated transmittance dependences on frequency demonstrating asymmetric (a) and symmetric (s) Fano resonances. Inset: the schematical view of the unit cell of the metasurface. The electric field of the electromagnetic wave is parallel to the *y*-direction, L_x=2L_y, and *d* denotes the thickness of the dielectric substrate.

Self-arrangement of nanostructured graphene films during plasma enhanced chemical vapour deposition (PECVD)

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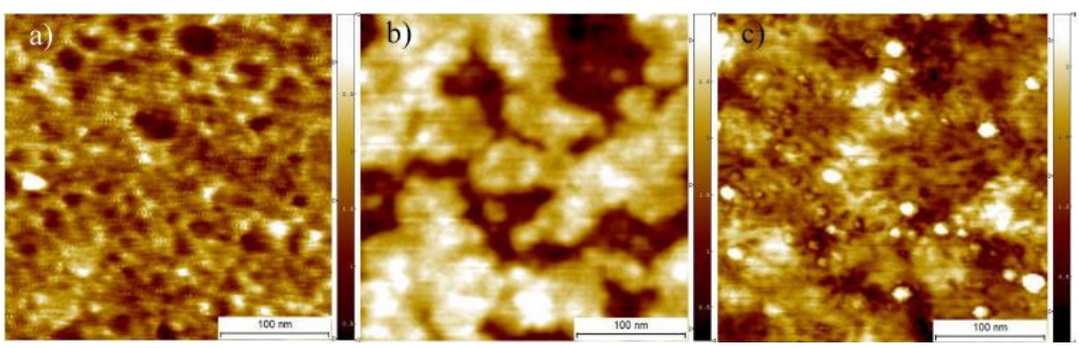
The method of graphene growth by PECVD was modified to exclude the influence of the energy gained by the ions in the accelerating electrical field. Our results proved that the effect of the etching by surface hitting ions can be efficiently reduced by placing the surface plane of the sample parallel to the plasma electric field. This approach eliminated point defects from the graphene cell. The growth dynamics was experimentally characterized by the AFM topography, height distribution and Minkowski connectivity. The most essential results are illustrated in Fig. 2 for the nano-crystalline graphene films grown at 550°C. The thickness of the films was 1 and 2 monolayers. An increase in the graphene flake diameter was due to increase in the amount of the non-accelerated ionized species hitting the surface area without noticeable increase in the surface roughness. It was concluded that the growth was controlled by the surface diffusion of the adatoms even at comparatively low temperatures (< 550 °C).

https://doi.org/10.1116/6.0002694



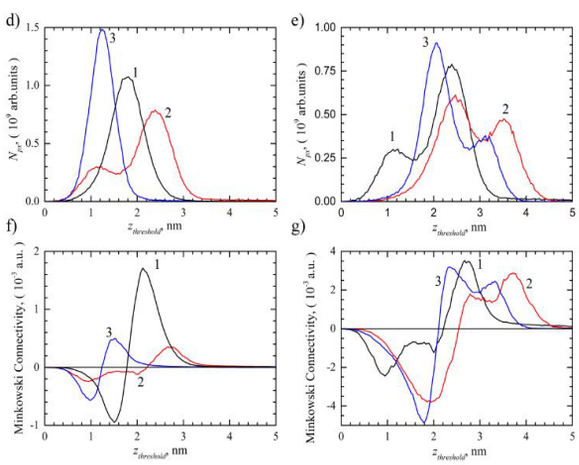


Fig. 2. (a-c) AFM topography images; (d, e) height distributions; (f, g) Minkowski connectivity for the nano-crystalline graphene grown by PECVD on SiO_2/Si substrates placed at distances 3.5 cm (a and 1 in (d-g)), 4.0 cm (b and 2 in (d-g)) and 4.5 cm (c and 3 in (d-g)) from the plasma edge at deposition temperature 550°C.

Department of Textile Technologies

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The highly qualified and experienced scientific team of the Department of Textile Technologies is involved in developing advanced textile technologies and high value-added products using novel fibers, new material structures and innovative textile finishing technologies. The Department is working actively at the international level. The project "ACROSS - Adaptive Camouflage for soldiers and vehicles", which has recently received funding approval from the European Defence Fund is based on collaboration with well-known research institutions and industry companies from nine EU countries and is the significant input in the international recognition of the FTMC. Our Department keeps close cooperation with the national industry as well. The R&D projects, a wide range of services is an integral part of our activities. The equipment of the Department of Textile Technologies is continuously renewed to meet the challenges of innovation-oriented research and reinforce the competitiveness of the FTMC.

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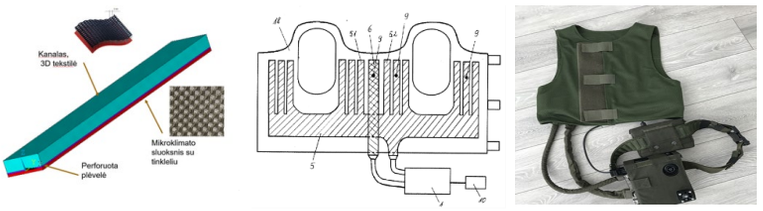
System and method for personal thermal comfort

We presented the invention of the system and the method for personal thermal comfort providing extra cooling or heating effect to users' body part area. The prototype of the mesh vest with integrated system for personal thermal comfort has been created. It can be worn as a separate garment or in conjunction with another garment, for example a ballistic vest or other protective garment (for motorcyclists, industry workers, etc.). The operating principle of

the system is based on a forced ventilated air movement within integrated two frameworks of 3D spacer textile channels: for ambient air distribution and for distribution of ambient, extra cooled or heated air flow. The extra cooling / heating is obtained using integrated thermoelectric elements working on a basis of the Peltier effect.



European Unitary Patent No. EP 4074206 "System and method for personal thermal comfort" by A. Abraitienė, D. Kubilienė, M. Šapurov, A. Dervinis, V. Bleizgys, A. Baškys and R. Bučas (2023 08 09).

Combined micro- and macro-scale modeling of heat and mass transfer through textile structures with additional ventilation

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The computational models of heat and mass exchange through textile structures with additional ventilation at the micro- and macro-scale were investigated. The finite element analysis of advanced textile materials provides a better understanding of their heat and mass transfer properties, which influence thermal comfort. The developed computational models can predict air permeability, thermal resistance, and heat transfer coefficients at the micro-scale. The mesh size was taken into consideration and validated with experimental data presented in the literature. The computational models were extended to micro- and macro-scale forced ventilation models. Macro-scale finite element models require input parameters such as an effective heat transfer coefficient that are usually obtained experimentally. We obtained the heat transfer coefficients numerically from the micro-scale model and applied to a macro-scale model. The proposed methodology and developed models allow to determine average temperature and temperature distributions through different through-thickness positions along the z-axis. The simulations were carried out using Comsol Multiphysics and Matlab software.

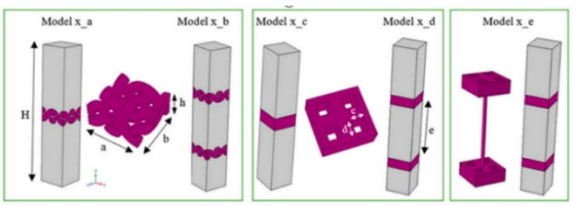

Fig. 1. The schematics of representative volume element of a 3D fabric.

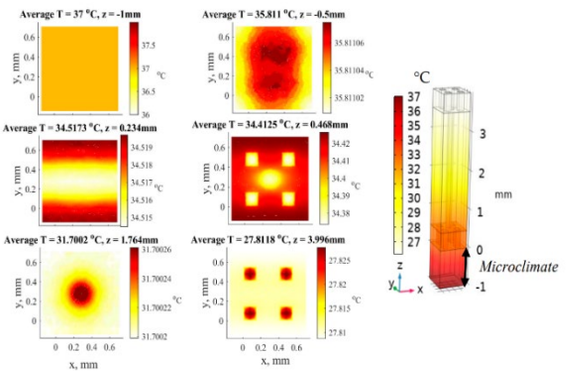

Fig. 2. Temperature distribution over the height of a representative volume element.

https://www.mdpi.com/2227-7390/11/11/2532

Investigation of electrical and wearing properties of wool fabric coated with PEDOT:PSS

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The research was aimed to enhance the wear resistance of a PEDOT:PSS coating on a wool fabric without reducing its electrical conductivity. This was achieved by introducing a low-formaldehyde-content melamine resin into the printing paste. The hydrophilicity and dyeability of wool fabric were improved through low-pressure nitrogen gas plasma modification. Two PEDOT:PSS dispersions were applied using exhaust dyeing and screen printing methods. Spectrophotometric analysis revealed that N2 plasma-modified samples exhibited more intense colour. SEM images showed deeper dye penetration after plasma modification. The HT coating appeared more homogeneous and uniform with a Tubicoat fixing agent (Fig. 3). The spectra of the chemical structure of wool fabrics coated with PEDOT:PSS were studied using FTIR-ATR (Fig. 4). The addition of melamine formaldehyde resins did not significantly decrease electrical conductivity, and the best results were obtained for samples subjected to the combined processing with N2 plasma modification, the exhaust dyeing with PEDOT:PSS, and the screen printing with a mixture of 3 wt.% melamine formaldehyde resins.

https://doi.org/ 10.3390/polym15112539

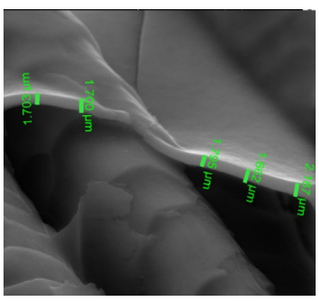


Fig. 3. SEM images of the wool fiber cross-section sample (PFSH) N_2 plasma-treated Clevios F ET dyed and Clevios S V3 with Tubicoat fixing agent HT screen printing method coating; magnification 5000×.

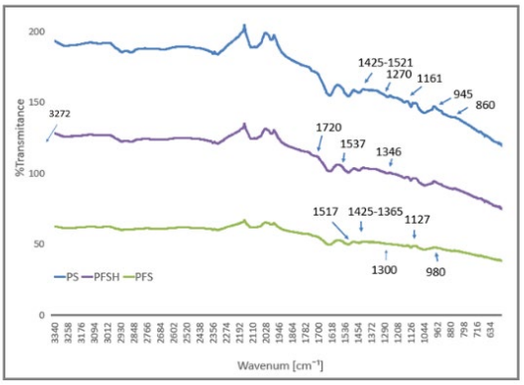
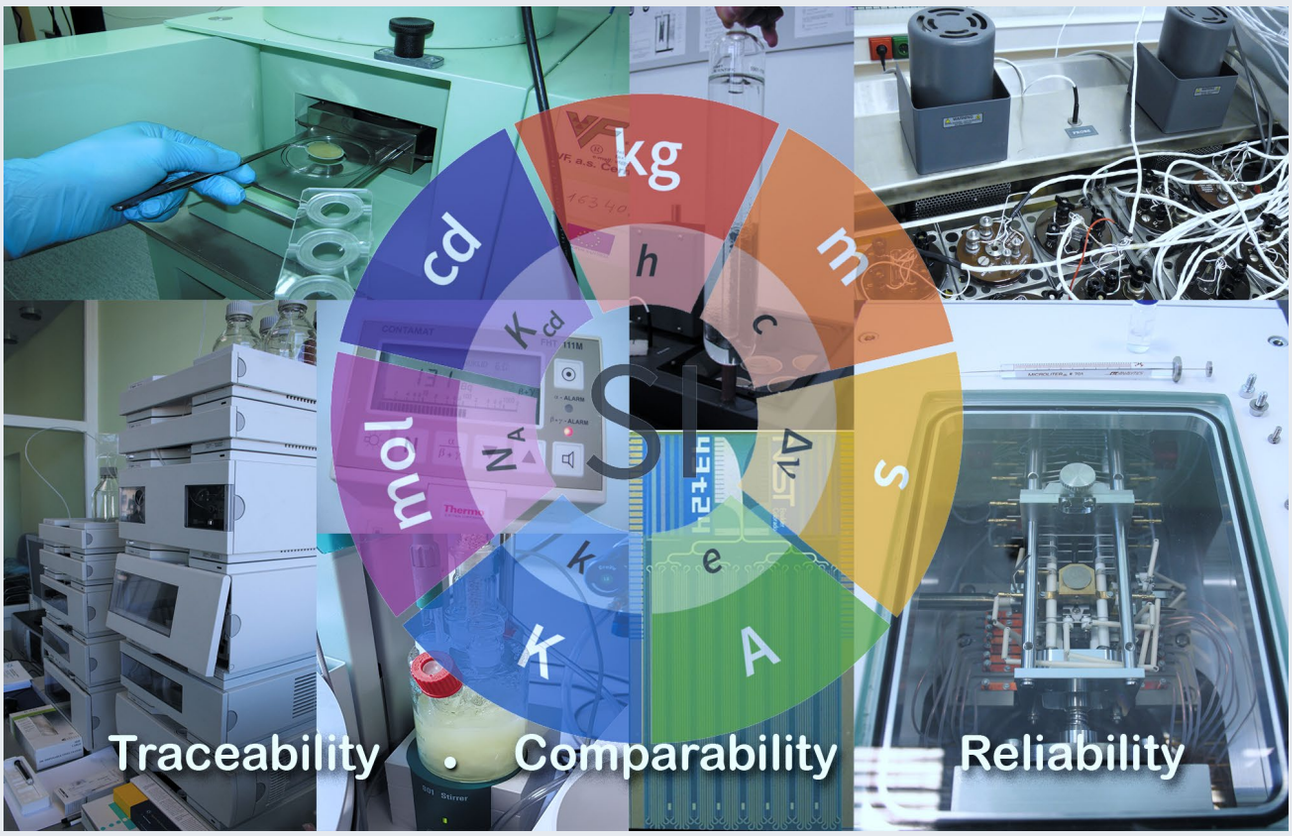


Fig. 4. FTIR-ATR infrared spectra of the wool samples PS, PFS, and PFSH.



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 17025:2018. 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 *Smart Specialisation in Northern Europe.* In 2023, FTMC joined the European Metrology Network *Pollution Monitoring*.

Currently, FTMC maintains the national standards in the seven 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 is issuing up to two million time stamps per month for Lithuanian governmental organisations and European users.

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

The mission of the **Temperature Unit Standard Laboratory (TUSL)** is 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 system. Lithuanian National Standard of the temperature unit (in the range from -195°C to +961,78° C) is of the primary level, while the reference point of the freezing point of Cu (+1084,62 °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 to maintain and transfer 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 to maintain and develop the standards of mass unit ensuring the traceability to the SI system in the range from 1 mg to 20 kg.

The reliable, traceable and accurate chemical measurements in different sectors of biotechnology, healthcare, safety and environment protection are provided by the staff of the NMI. The 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* are continued. The project develops prototypes for new products characterizing chemical compounds applied in chemistry, cosmetics and pharmaceutical industry. Another area of interests of NMI is a new regional metrological capacity for certification of reference materials according to the requirements of ISO 17034 standard.

The **Ionizing Radiation Metrology Laboratory (IRML)** of NMI organized the international comparison piloted by the FTMC for EURAMET.RI(II)-S9 *The third interlaboratory comparison of the radionuclide calibrators*. The Laboratory also continued its planned activities within the EMPIR 2020 joint research project 20SIP02 *FreeRelease* 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, have been 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 MoS2, 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^2) 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 nanostructures 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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Converse and chemical coatings 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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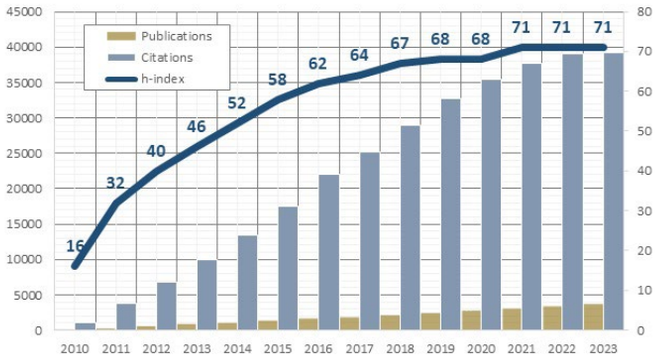
In the new microwave anechoic chamber, we developed a setup for microwave transmission and reflection measurement in a frequency range from 1 GHz to 18 GHz. Measured sample is placed in the aperture of the absorbing panel. Using this technique, it is possible to measure microwave properties of various modern materials: windowpanes, absorbing textiles, shielding materials, etc.

Publications

Evolution of publications with FTMC affiliation, citation rates and H index in 2010-2023



*data according to Web of Science

With FTMC affiliations in 2023 in the top quartiles (Q1-Q2) journals

1. **Abedivaraki, M.**; Daraei, M.E. Impact of wiggler magnetic field on wakefield generation and electron acceleration by Gaussian, super-Gaussian and Bessel–Gaussian laser pulses propagating in collisionless plasma // Journal of plasma physics. New York : Cambridge University Press (CUP). ISSN 0022-3778. 2023, vol. 89, iss. 1, art. no. 905890114, p. 1-16.

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12. **Astrauskytė, D.**; Galvanauskas, K.; Gailevičius, D.; **Drazdys, M.**; Malinauskas, M.; **Grinevičiūtė, L**. Anti-reflective coatings produced via atomic layer deposition for hybrid polymer 3D micro-optics // Nanomaterials. Basel : MDPI. eISSN 2079-4991. 2023, vol. 13, iss. 16, art. no. 2281, p. 1-13.

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