CENTER
FOR PHYSICAL SCIENCES
AND TECHNOLOGY

ANNUAL REPORT 2024

CENTER FOR PHYSICAL SCIENCES AND TECHNOLOGY (FTMC)

is the largest scientific research institution carrying out a unique fundamental research and technological development works in scientific fields of laser technologies, optoelectronics, nuclear physics, organic chemistry, bio and nanotechnologies, electrochemical material science, functional materials, electronics, etc. in Lithuania. In the Center not only the innovative science but also high technologies expedient for business and society needs are developed.

OUR MISSION

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

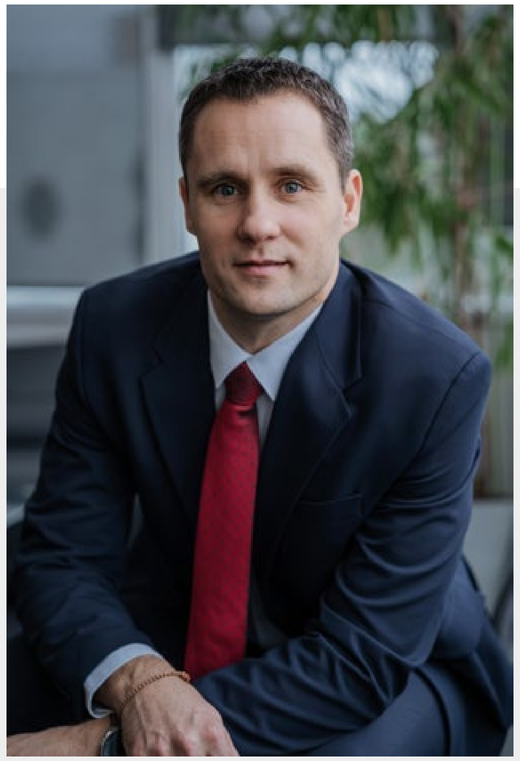
OUR MOTTO

Be inventive.

OUR VISION

FTMC among the best science and technology organisations.

CONTENTS



THE MESSAGE FROM THE DIRECTOR:

THE YEAR OF 2024: A YEAR IN TRANSITION AND NEW HORIZONS

This has been a year of change for FTMC, including my taking over as Director. In this first annual message, I look back on a year in which our institution was able to build on its strengths and further develop its identity.

In our pursuit of strategic developments, we prioritise our international visibility and greater opportunities for collaboration in cutting-edge research. In this context, I am pleased to recognise the continued efforts to strengthen ties with Taiwan and South Korea, particularly sharing in the area of electronics development. Given the rising global demand for semiconductors and the EU's initiatives, such as the Chips Act and the Chips Competence Centres, FTMC is committed to advancing these research areas. Our impact and presence in the research ecosystem will depend on our drive to excel further. Engaging with international networks, such as the European Association of Research and Technology Organisations (EARTO), the European Photonics Industry Consortium (EPIC), and the European Physical Society (EPS), as well as fostering new partnerships – such as our recent inclusion in the Advanced Material Initiative (AMI)) – will be crucial. Being part of these networks provides unique opportunities FTMC researchers must actively pursue to translate them into impactful outcomes or to bolster emerging strengths, particularly by focusing our efforts on chips and quantum research.

Our local partnerships demonstrate FTMC's ability to strengthen Lithuania's public and private sectors through applied research. In particular, in 2024, we have contributed to the expansion of the energy sector through novel applications of our scientific expertise, including the development of microbial fuel cells and green hydrogen. Laser technologies remain one of FTMC's core strengths. Specifically, I highlight the identification of new research application sectors, such as the use of these technologies in the defence sector. I strongly believe that FTMC's collective value outweighs the sum of its individual parts, and that the most successful outcomes will be achieved through mutual trust and collaboration among our scientific departments, industry, government, commercialisation team and other stakeholders in the research ecosystem. The recent meeting with senior officials from the Lithuanian armed forces highlights how continued research into military technologies has led to opportunities for long-term partnerships of both national and international importance. In all areas of our research, the pathway forward should focus on key sectors where FTMC can make meaningful, lasting contributions that enhance our presence as a research institute.

I would like to take this opportunity to commend the FTMC researchers who have been recognised for their excellence in research throughout the year. Some highlights include the Lithuanian Science Prize in the natural sciences (awarded by the Lithuanian Academy of Sciences) and the Presidential Order of the Lithuanian Grand Duke Gediminas (for accomplishments in advancing biophysics). In 2024, FTMC researchers authored over 200 scientific papers published in internationally recognised journals, with several standout achievements marking the excellence of their work. Their research have been featured in prestigious journals, such as *Laser & Photonics Reviews, Advanced Optical Materials, and Advanced Engineering Materials*. As we celebrate these achievements, I want to emphasise that the impact of FTMC is a collective effort, with each scientific division contributing to our overall standing in the Lithuanian research landscape.

Our young scientists remained engaged throughout the year, participating in international conferences and receiving recognition for their remarkable achievements. The year witnessed the successful defence of 17 dissertations, and I am pleased to note that a PhD student from FTMC was recognised as the author of the best PhD thesis in 2024. As an institution, we should strive for even greater impact on the next generation of scientists. To remain competitive and attract young talent eager to build their researcher careers, FTMC must develop a comprehensive approach through a doctoral school that fosters students on their PhD journey. This PhD school will be our focus going forward, adding value to our PhD students and ensuring research excellence and impact emerging from the future generation of researchers working at FTMC.

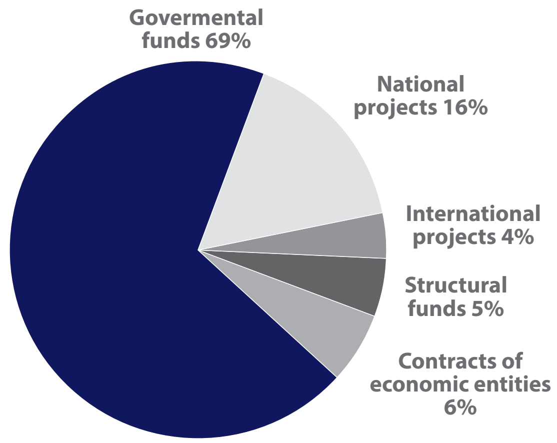
As 2024 comes to a close, I am pleased to reflect on a year in which this institution was an active participant in both national and international research. We must carry this momentum forward and continue expanding our horizons. It is only by maintaining an openness to change that we can progress towards the next stage of research excellence at FTMC.

RAMŪNAS SKAUDŽIUS
Vilnius, 2024

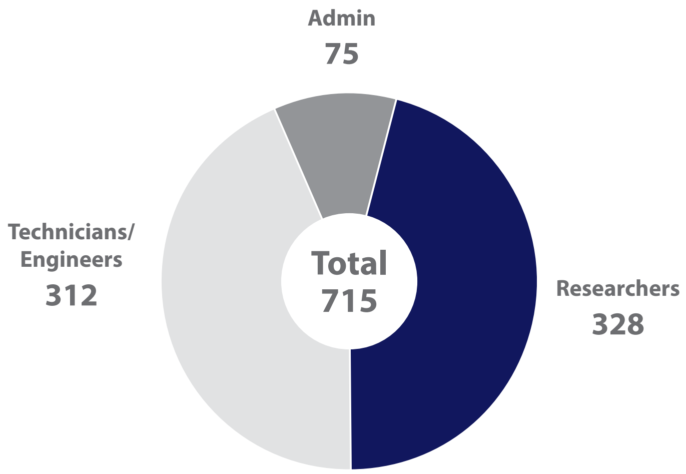
FACTS & FIGURES

FTMC Budget, kEur

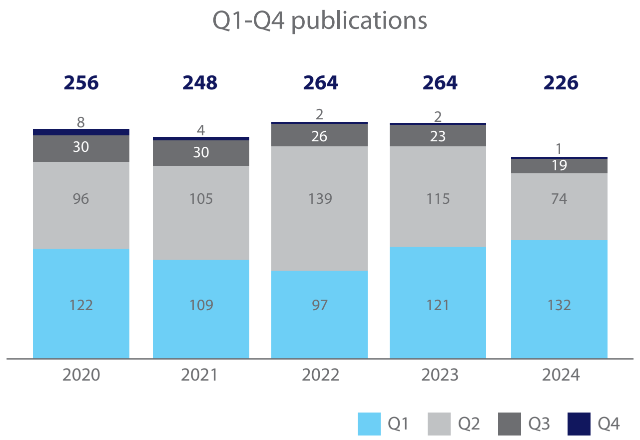
	2023	2024
Govermental funds	16447,0	19028,5
National projects	3191,6	4431,3
International projects	269,4	1086,6
Structural funds	2995,8	1381,3
Contracts of economic entities	2951,0	1818,2
TOTAL:	25854,85	27745,9



FTMC Staff

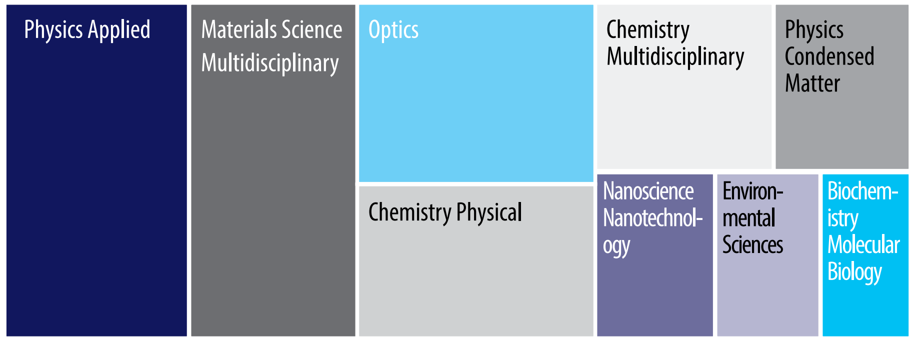


FTMC publications



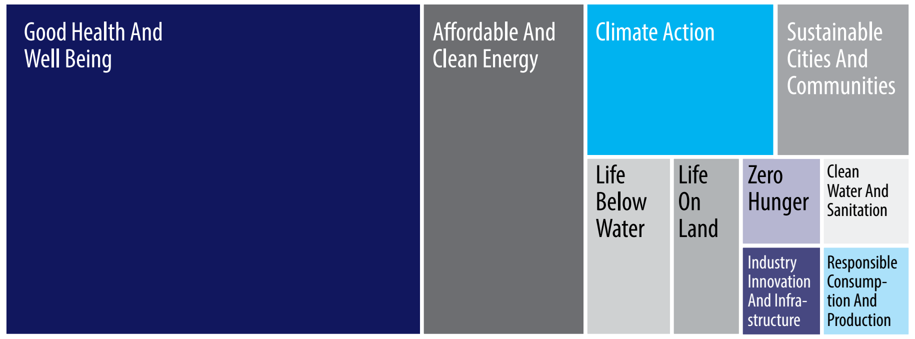
Following half a decade of high scientific output, in 2024 FTMC marks a period of transition and opportunities for scientists to examine new prospects of scientific inquiry and potential for breakthrough innovations.

FTMC publications in 2024 by Web of Science Categories



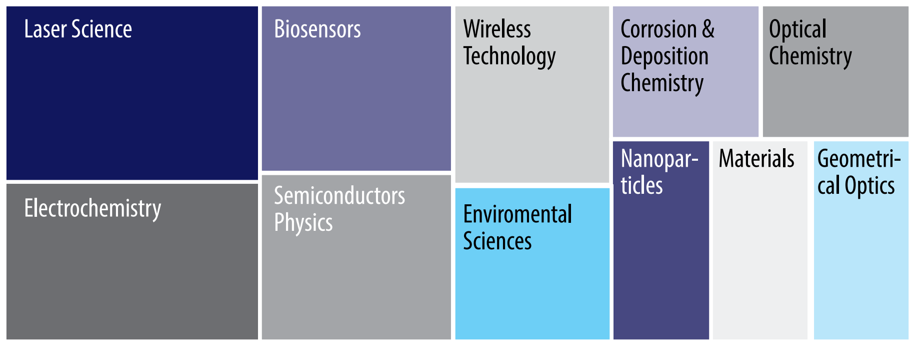
In 2024 FTMC scientists focused on research in applied physics and chemistry, with considerable input towards advancing discoveries in material sciences. We also note the impacts towards nanoscience, nanotechnology as well as environmental sciences, the later showcasing FTMC contribution towards solving common European challenges emerging from the green transition.

FTMC publications contributing to Sustainable Development Goals in 2024



It is important to note how the publication from FTMC were aligned with wider societal challenges. Research in 2024 contributed towards innovations in affordable and clean energy and achieving positive contributions towards climate actions. These topics are of major interest in several of FTMC research departments with goals to continue exploring research supporting these Sustainable Development Goals. Most importantly, FTMC researchers conducted scientific work advancing good health and wellbeing, signalling potential of FTMC research outputs in medical application.

FTMC publications in 2024 by Web of Science Citation Topics Meso



Further examination of research conducted in 2024 demonstrates the prevailing role laser science where our scientific departments have continued striving to be on the cutting edge of technological development. Within FTMC scientists benefit from synergies between different scientific divisions – revealed through publications in electrochemistry, biosensors, semiconductors and optics. This comprehensive access to interconnected research in photonics will be utilised in the future, ensuring a robust research value chain where fundamental research enquiries run parallel to practical application of science that benefits Lithuania and our international partners.

It is important to acknowledge the lowered publishing of scientific papers and patent applications when compared to prior years. It is equally important to contextualise these numbers as the closing of one chapter of FTMC history and the beginning of a new one. Our scientific divisions (presented in greater detail through dedicated chapters further in this report) are analysing new research directions where the scientific potential accumulated within FTMC would be best directed. The responsibility to utilise this potential effectively lies with the scientists of FTMC.

DOCTORAL THESES

PHYSICS

MATAS RUDZIKAS
Investigation of optical and electrical characteristics in photovoltaic devices colored by the functional metal oxide coatings.
Scientific supervisor: dr. A. Šetkus

TOMAS DAUGALAS
Investigation of dependence of electrical properties on external mechanical force and electrical field in a structure with graphene sheet separating surfaces of conductors.
Scientific supervisor: dr. A. Šetkus

ALGIMANTAS LUKŠA
Investigation of the properties of graphene layers on insulating substrates: their dependence on growth conditions and interaction with humidity.
Scientific supervisor: dr. A. Šetkus

PAULIUS ŠLEVAS
Methods for the formation of structured light beams and their application for laser microprocessing.
Scientific supervisor: dr. S. Orlovas

JUSTINAS JORUDAS
Optical and Electrical Investigation of GaN-based HEMT and Graphene Structures for Applications in THz Detection.
Scientific supervisor: dr. I. Kašalynas

MARIUS ČEPONIS
Stellar populations in low mass systems.
Scientific supervisor: prof., dr. V. Vansevičius

DANIIL PASHNEV
Stellar populations in low mass systems.
Scientific supervisor: dr. I. Kašalynas

VLADISLOVAS ČIŽAS
Coexistence of high-frequency parametric and Bloch gain in doped GaAs/AlGaAs superlattices.
Scientific supervisor: prof., habil. dr. G. Valušis

CHEMISTRY

VAIDAS PUDŽAITIS
Surface enhanced infrared absorption spectroscopy of biomolecular layers and water at gold surface.
Scientific supervisor: prof. habil. dr. G. Niaura

KATSIARYNA CHARNIAKOVA
Synthesis and characterization of functional coatings and nanoparticles.
Scientific supervisor: dr. A. Jagminas

ANTANAS NACYS
New materials for low temperature fuel cells.
Scientific supervisor: dr. L. Tamašauskaitė-Tamašiūnaitė

RAIMONDA BOGUŽAITĖ
Development of an electrochemical sensor based on polypyrrole and modification of its properties.
Scientific supervisor: dr. V. Ratautaitė

MARYIA DROBYSH
Electrochemical biosensors for COVID-19 diagnosis.
Scientific supervisor: prof., habil. dr. A. Ramanavičius

EDITH FLORA JOEL
Investigation of chitosan-graphene oxide nanocomposites and their application in environmental protection.
Scientific supervisor: dr. G. Lujanienė

MATERIAL ENGINEERING

GUSTAS LIAUGMINAS
Nonlinear pulse formation in an optical fibers.
Scientific supervisor: dr. K. Regelskis

ROMUALD PETKEVIČ
Development and application of laser metal particles sintering technology.
Scientific supervisor: dr. G. Mordas

KAROLIS STAŠYS
Strategies for developing innovative mid-infrared light sources using molecular beam epitaxy.
Scientific supervisor: dr. J. Devenson

SIMAS MELNIKAS
Investigation of dependence of Bragg and chirped mirrors design to spectral parameters and optical resistance.
Scientific supervisor: dr. R. Drazdys

ABOUT PHD STUDIES

As part of our ongoing commitment to enhancing the doctoral program, we aim to increase the number of doctoral students by attracting more candidates from developed economies as defined in the **World Economic Situation and Prospects (WESP)** report. Currently, only **7% of our international doctoral students** come from WESP-developed economies, underscoring a significant opportunity for growth in this area.

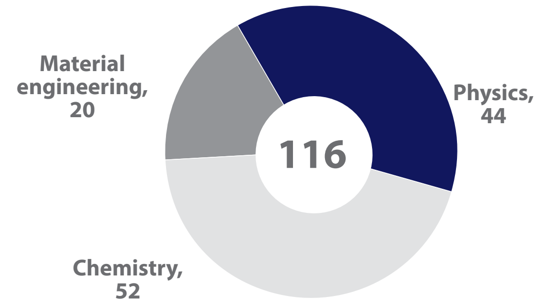
While there was a slight dip in the total number of doctoral students in 2023, the admissions and dissertation defenses in 2024 indicate promising growth. To sustain and amplify this trend, we plan to implement targeted recruitment strategies and collaborations aimed at attracting talented students from WESP-developed economies.

Additionally, we are proud to share that our doctoral program has been recognized for excellence, with one of our dissertations winning the **BEST DISSERTATION AWARD** for three consecutive years. This achievement reflects the dedication and high standards of both our doctoral candidates and faculty.

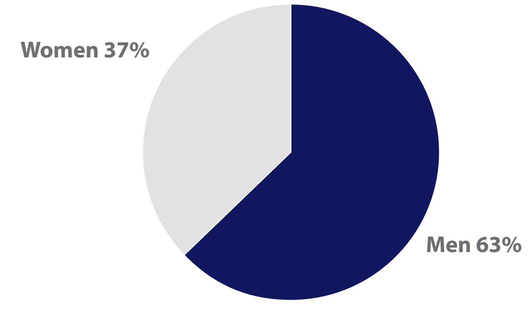
Looking ahead, one of our strategic goals for 2025 is the establishment of a Doctoral School. This initiative aims to provide a structured framework for doctoral studies, fostering interdisciplinary collaboration, enhancing academic support, and further strengthening the international appeal of our program.

We remain committed to fostering a globally diverse academic community and raising the profile of our doctoral program on the international stage.

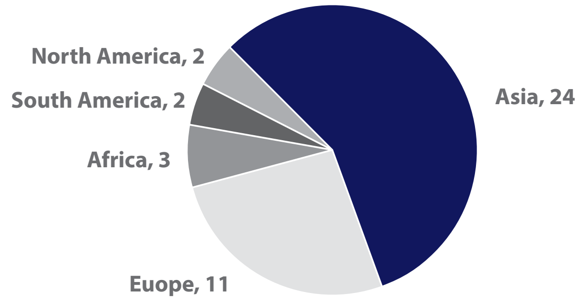
PhD students in total



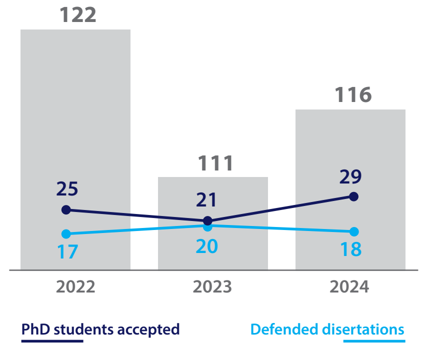
PhD students by gender



PhD students from foreign ountries



Number of PhD students



MAIN INTERNATIONAL PROJECTS IN 2024

European Commission Project
European Joint Research Programme In The Management And Disposal Of Radioactive Waste, EURAD. 2019-2024
Rita Plukienė

Horizon 2020 Programme Project
Pre-Disposal Management Of Radioactive Waste, PREDIS. 2020-2024
Rita Plukienė

Horizon 2020 Programme Project
Fostering The PAN-European Infrastructure For Empowering SMEs Digital Competences In Laser-Based Advanced And Additive Manufacturing, PULSATE. 2020-2024
Gediminas Račiukaitis

Horizon 2020 Programme Project
Laser-Plasma Based Source 3D Tomography For Cargo Inspection, MULTISCAN 3D. 2021-2025
Gediminas Račiukaitis

Horizon 2020 Programme Project
Innovation Fostering In Accelerator Science And Technology, I.FAST. 2021-2025
Vidmantas Tomkus

Horizon 2020 Programme Project
Sustainable Self-Charging Power Systems Developed By INKjet Printing, SUINK. 2024-2026
Gediminas Račiukaitis

Research Executive Agency (REA) Project
Terahertz Photonics For Communications, Space, Security, Radio-Astronomy, And Material Science, TERAOPTICS. 2020-2024
Irmantas Kašalynas

Research Executive Agency (REA) Project
Fluorescent NanO-Agents For Super-Resolution Imaging And Sensing, FLORIN. 2022-2026
Renata Karpič

European Health And Digital Executive Agency Project
Evidence Driven Indoor Air Quality Improvement, EDIAQI. 2022-2026
Steigvilė Byčenkienė

European Defence Fund Project
Additive Manufacturing Of Lightweight Laser Target Designator, AMLTD. 2022-2026
Genrik Mordas

SPS Programme Project
3D Metamaterials For Energy Harvesting And Electomagnetic Sensing. 2023-2026
Žilvinas Andrius Kancleris

European Commission Project
Adaptive Camouflage For Soldiers And Vehicles, ACROSS. 2023-2027
Julija Baltušnikaitė-Guzaitienė

European Commission EURATOM Project
European Partnership On Radioactive Waste Management 2, EURAD-2. 2024-2029
Artūras Plukis

European Space Agency Project
Force Spectroscopy Of Microtissues For Direct Probing Of Microgravity Effects. 2024-2027
Artūras Ulčinas

European Space Agency Project
Development Of The Beta-BBO Crystal Growth Technology For European Laser Industry. 2024-2025
Martynas Misevičius

PROJECTS PARTNERS

BUSINESS PARTNERS

FTMC researchers offer their scientific competence, suitable working facilities, and other research and experimental services to scientific institutions and business partners. This activity results in scientific research performed under contracts with various Lithuanian and foreign companies.

INTERNATIONAL PATENTS 2020-2024

2020

Pretreatment Of Plastic Surfaces For Metallization To Improve Adhesion
US 10526709 B2
Karolis Ratautas, Gediminas Račiukaitis, Aldona Jagminienė, Ina Stankevičienė, Eugenijus Norkus

Method For Formation Of Electro-Conductive Traces On Polymeric Article Surface
US 10982328 B2
Karolis Ratautas, Gediminas Račiukaitis, Aldona Jagminienė, Ina Stankevičienė, Eugenijus Norkus

Sensor For Electromagnetic Radiation Of Microwave And Terahertz Frequencies
EP 3582269 B1
Algirdas Sužiedėlis, Steponas Ašmontas, Jonas Gradauskas, Angelė Danutė Steikūnienė, Gytis Julius Steikūnas, Maksimas Anbinderis

2021

Method And Device For Sum-Frequency Generation Of Light Pulses
EP 2621032 B1
Kęstutis Regelskis, Julijanas Želudevičius, Gediminas Račiukaitis

Method For Formation Of Electro-Conductive Traces On Polymeric Article Surface
US 10982328 B2
Karolis Ratautas, Gediminas Račiukaitis, Aldona Jagminienė, Ina Stankevičienė, Eugenijus Norkus

Chrome-Free Adhesion Pre-Treatment For Plastics
US 10920321 B2
Mark Hyman, Leonas Naruškevičius, Danas Budilovskis

2022

Low Contact Resistance Device And Method Of Production
EP3840050B1
Steponas Ašmontas, Jonas Gradauskas, Konstantinas Leinartas, Laurynas Staišiūnas, Algirdas Sužiedėlis, Aldis Šilėnas

Method For Fabrication Of Recessed Electrical Elements
EP3975224B1
Irmantas Kašalynas, Simonas Indrišiūnas, Pawel Prystawko, Piotr Kruszewski

2023

Method Of Polymethylmethacrylate (PMMA) Removal From A Graphene Surface By Photoexposure
EP 3936476 B1
Natalia Alexeeva, Irmantas Kašalynas

System And Method For Personal Thermal Comfort
EP 4074206 B1
Aušra Abraitienė, Diana Kubilienė, Martynas Šapurov, Aldas Dervinis, Vytautas Bleizgys, Algirdas Baškys, Remigijus Bučas

2024

Manufacture Of Electro-Magnetic Shielding Textiles With Conductive Organic Polymeric Coating
EP 3854933 B1
Aušra Abraitienė, Audronė Sankauskaitė, Vitalija Rubežienė

Method For Batch Processing Of 3d Objects Using Laser Treatment And A System Implementing The Method
EP 4043142 B1
Gediminas Račiukaitis, Karolis Ratautas, Vytautas Vosylius

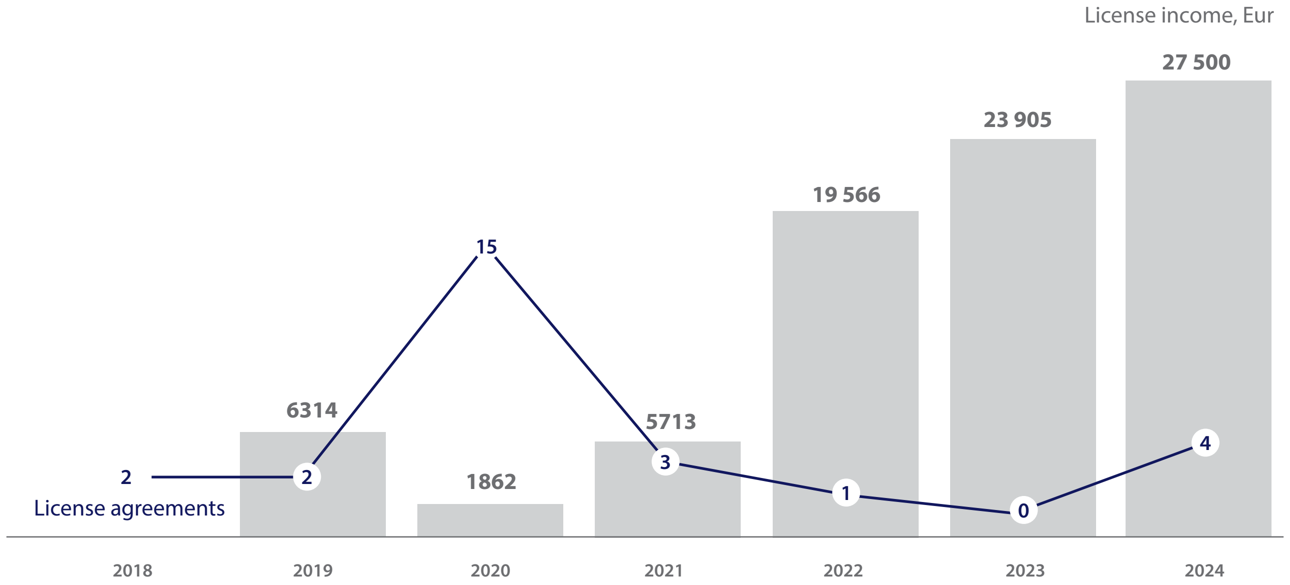
LICENSE AGREEMENTS 2024

Plasmonic Sensor To Determine Fibronectin Concentration,
MB "Optiniai Instrumentai"

Wetting Angle Measurement System,
MB "Femto nano bio"

Laser Processing Method For The Production Of Optical Components Of Transparent Materials,
UAB "Rocker Optics"

Efficient Laser Beam Splitter,
MB "Nanofotonika"



The 2024 licence agreements showcase renewed interest from private companies to utilise FTMC expertise in applied photonics. This marks the first time since 2020 when we experience growth in licence agreements, following the significant jump of licences in 2020 resulting from successfull MITA funding grants. The licence agreements in 2024 demonstrate FTMC our continued efforts in exploring new application of our scientific discoveries and building relationships with private sector partners.

OPEN ACCESS FACILITIES

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

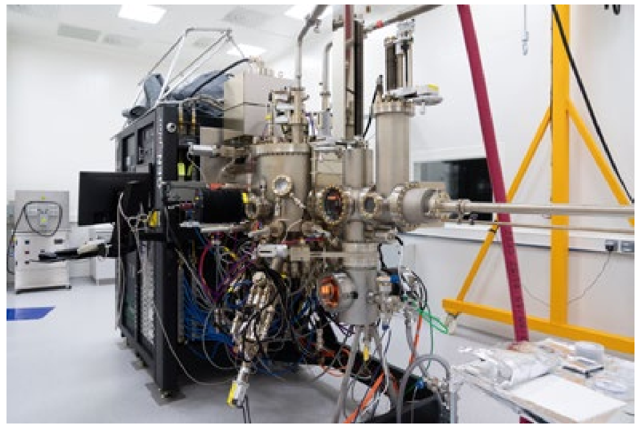
https://litexbeam.ftmc.lt

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 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.

Microwave transmission, reflection and absorption

paulius.ragulis@ftmc.lt

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.



Prototype formation and integration

karolis.stasys@ftmc.lt

Clean room technology for prototyping of semiconductor-based devices

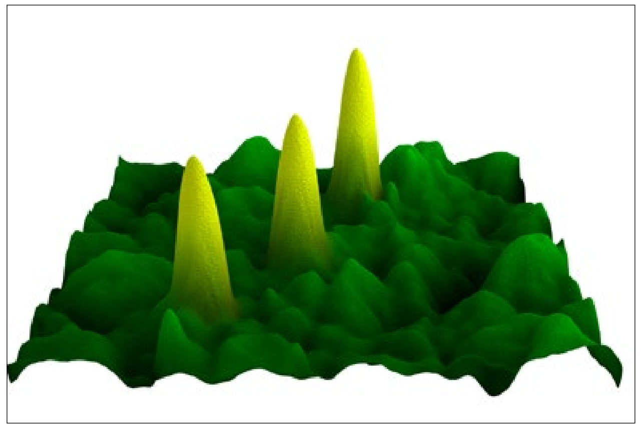
Based on a collaboration between the Departments for Physical Technologies and Optoelectronics, a complete cycle of the clean room (CR) micro-processing line has started to function. It is ready to produce the working models and the demonstration proto-types of chemical and photo-sensitive devices as 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 m2) operations, 2) photolithography, 3) laser lithography, 4) wet chemical processing, 5) thermal processing, 6) metal and oxide coatings, 7) assemblage and testing.

Characterisation and testing of prototypes

The R&D projects in the 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.

AWARDS

DR. ARŪNAS JAGMINAS, a researcher at the Department of Electrochemical Material Science of FTMC, has been awarded the 2023 Lithuanian Science Prize in the field of natural sciences. He was honored for his work "Studies into the Formation, Characterisation, and Applications of Marketable Nanostructures (2007-2021)".

A. Jagminas found and applied the new methods of electrochemical, thermal or hydrothermal synthesis of various metals, semiconductors, hybrid nanoderivatives and their ordered colonies. "This award is not just an appreciation of my work, told the researcher, this is a recognition of all the works and results achieved by our Center during those years."

DR. IEVA PLIKUSIENĖ, a researcher at the Department of Nanotechnologies of FTMC, has been awarded the Medal of the Order of Grand Duke Gediminas of Lithuania. She was distinguished for the highest international level research in biotechnology, her significant contribution to the progress of science in various fields, and for promoting Lithuania in the world.

"This is probably my most significant recognition, told Ieva, because I consider contributing to the development of science in Lithuania, where I was born and grew up, the greatest value. Although a lot of scientific research has been done with colleagues from abroad, all my papers are attributed to Lithuanian institutions, Vilnius University and FTMC."

HABIL. DR. EVALDAS TORNAU, a researcher at the FTMC Department of Functional Materials and Electronics, has been awarded the Knight's cross of the Order of Grand Duke Gediminas of Lithuania. E. Tornau is a theoretical physicist whose scientific interests are mostly related to phase transition models in different materials. He is a laureate of the Lithuanian Science Prize (2002) and a long-time editor of the Lithuanian Journal of Physics.

DR. GINTARĖ GEČĖ, a researcher at the Department of Chemical Engineering and Technology of FTMC is the author of the best PhD thesis in 2023. Her thesis "Search, Synthesis, and Investigation of New Framework Electrode Materials for Aqueous Na-ion Batteries" was evaluated in the nature, technology, medicine and health and agricultural sciences category. The Best Dissertation Competition is organized annually by the Lithuanian Union of Young Scientists. For the third year in a row, the winners of this competition are young scientists from FTMC.

DR. ANDREJUS MICHAILOVAS, a researcher at the Department of Laser Technologies of FTMC – among the world's top 100 photonics leaders!

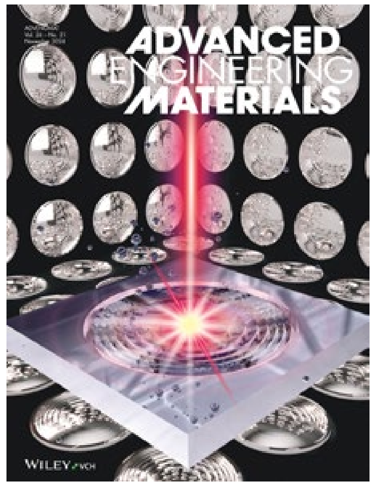
Three years in row Electro Optics magazine has ranked the world's top 100 photonics leaders. Among scientists, inventors, industry representatives and start-ups from the USA, Germany, India, South Africa and other countries, A. Michailovas is the only one nominee from Lithuania.

DR. ANDRIUS ŽEMAITIS, a researcher at the Department of Laser Technologies of FTMC, became the laureate of the Lithuanian Academy of Sciences Young Scientists Scholarship Competition in the field of technological sciences for his research "Development of high-performance laser micromachining technologies for creating functional surfaces".

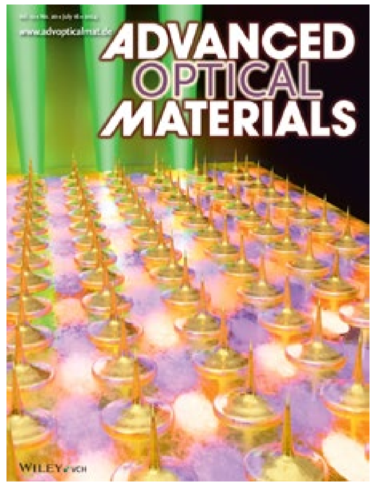
DR. ROKAS KONDROTAS, a researcher at the Department of Characterisation of Materials Structure of FTMC, was elected as a new member of the Mathematics, Physics and Chemistry Division of the Young Academy of the Lithuanian Academy of Sciences.

DR. MINDAUGAS GEDVILAS, a researcher of the Department of Laser Technologies of FTMC, winner of the 2020 Lithuanian Science Prize, has become an Associate Editor of Optics Express. This journal is the world's most cited journal in optics. According to the Journal Citation Reports, it was cited 131,556 times in 2023, ranking first among 120 journals.

COVERS OF SCIENTIFIC JOURNALS



The paper "Efficient ablation, further GHz burst polishing, and surface texturing by ultrafast laser" by **Mindaugas Gedvilas, Andrius Žemaitis and Paulius Gečys** from Department of Laser Technologies of FTMC has been selected as the leading research paper for November in *Advanced Engineering Materials* journal. The illustration from this article was shown at the cover of the journal.



The researchers from FTMC, **Kernius Vilkevičius, Algirdas Selskis and Evaldas Stankevičius**, in collaboration with George D. Tsibidis and Emmanuel Stratakis from FORTH (Greece), have published a paper entitled "Formation of highly tunable periodic plasmonic structures on gold films using direct laser writing". The paper is published in prestigious journal *Advanced Optical Materials* in July 2024, and the illustration of this research features the cover of the issue.

The prestigious international scientific journal *Laser & Photonics Reviews* has selected a paper "Light Engineering and Silicon Diffractive Optics Assisted Nonparaxial Terahertz Imaging" by FTMC researchers **Sergej Orlov, Rusnė Ivaškevičiūtė-Povilauskienė, Karolis Mundrys, Paulius Kizevičius, Ernestas Nacius, Domas Jokubauskis, Kęstutis Ikamas, Alvydas Lisauskas, Linas Minkevičius, Gintaras Valušis** as the leading article, and its illustration was featured on the cover of the May 2024 issue.

An article entitled "MnO_2 nanoparticles supported on graphitic carbon nitride as an electrocatalyst for oxygen reduction and evolution", written by the FTMC researchers **Aušrinė Zabielaitė, Virginija Kepenienė, Dijana Šimkūnaitė, Raminta Stagniūnaitė, Vitalija Jasulaitienė, Giedrius Stalnionis, Jūratė Vaičiūnienė, Loreta Tamašauskaitė-Tamašiūnaitė, and Eugenijus Norkus**, has been selected as the lead research paper in the prestigious journal "New Journal of Chemistry", and its illustration has been featured the cover of the December 2024 issue.

EVENTS

14-15 February 2024

FTMC Annual Scientific Conference

At the conference, FTMC scientists presented their research results and highlighted their annual achievements.

30 May 2024

CleanTech Innovations

For the first time, FTMC, Baltic Sandbox Ventures, and the Cleantech Cluster Lithuania organized the CleanTech Innovations science and business forum. The event aimed to introduce the ecosystem of clean and renewable technologies within FTMC's research and technology development areas, while fostering collaboration among the forum's members.

5 April 2024

International Workshop on Laser Particle Accelerators: Applications and Experimental Possibilities at the ELI Infrastructure

Researchers and laser experts from the Czech Republic, Italy, Israel, Lithuania, Romania, and Hungary gathered to discuss and share insights on current opportunities to visit ELI facilities for testing next-generation lasers in experiments. This workshop served as an opportunity to invite world-renowned scientists in the field.

5 June 2024

PULSATE Connect: Laser Innovation for SMEs

Small and medium-sized enterprises were invited to the PULSATE Connect: Laser Innovation for SMEs event, which presented information about laser technologies and their positive impact on industry. Attendees also learned about available funding opportunities from the European Commission, established connections with professionals in the field, and analysed success stories of digital transformation in small and medium-sized enterprises.

11-14 June 2024

European Workshop on Innovative and Advanced Epitaxy

The workshop was held at the FTMC, where young scientists and invited guests presented their research on the topic. Epitaxy is the process of growing crystalline layers at the atomic level, one on top of another, which are then used to enhance semiconductor, light-emitting diode (LED), laser, quantum and other technologies. The workshop, along with the subsequent discussions, covered both theoretical and practical aspects of epitaxy research

1-6 July 2024

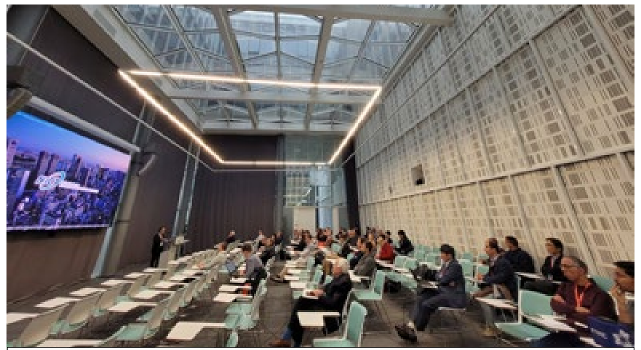
Summer School on Ultra-short Pulse Lasers Applications in Material Processing - UPLAMP 2024

The international school, featuring esteemed lecturers and engaging excursions, was designed for enthusiastic students and young researchers working in the field of ultra-short pulse laser applications in material processing

14-19 July 2024

International Traveling Summer School on Terahertz Sciences and Technology

Vilnius University and FTMC organized the International Traveling Summer School on Terahertz Sciences and Technology. The program included lectures on the latest achievements in terahertz technology and applications. The lectures were followed by discussions and interactions among students, professors, and industry professionals. The event also featured visits to companies, group challenges, diverse lab tours, and social events



1–4 October 2024

International scientific conference on Advanced Properties and Processes in Optoelectronic Materials and Systems - APROPOS 19.

The conference aimed to reveal and share new ideas in the technology, research, and applications of advanced optoelectronic materials. It sought to explore modern trends in optoelectronics research and to discuss the processes and fascinating phenomena that arise when optics meets electronics. Special emphasis was placed on the applications of ultrafast methods for advanced materials.

1 October 2024

Tutorial Session & Masterclass on Scientific Writing

This training, designed for PhD students, aimed to enhance their skills in scientific writing, publishing and presenting their research.

15–17 October 2024

14th Conference of Doctoral Students and Young Scientists – FizTech2024

At this annual conference, PhD students from FTMC presented the results of their research in physics, chemistry, and materials engineering.

FTMC SCIENTISTS AND THE POPULARIZATION OF SCIENCE

The question **SO WHAT ARE YOU DOING THERE?** is often heard by researchers working at the Center, and it is a very good time to respond to it in a FTMC podcast. Every second Thursday the physicists, chemists, experts in material science and electronics from FTMC present their current research and explain the benefits of their scientific discoveries for each of us in a simple and comprehensible way. There is no shortage of interesting topics in the FTMC, the largest scientific research institution in the Baltic States. "The Power of Theoretical Physics", "What We Don't Know About the Universe", "Lasers and Shark Skin", "Trees, Mammoths and Radioactive Carbon", "Radioactive Particle Research" are just a few examples of what we talk about.

Physicists, chemists, and materials engineers from FTMC conduct extremely interesting and significant research which is important for all of us. However, these works are often invisible to general public. Throughout the autumn, open discussions **INSPIRED BY SCIENCE** were held in the Museum of Energy and Technology. Fourteen FTMC researchers shared their knowledge with general audience and visually presented how science works - what is happening in our laboratories and what amazing ideas are born in the heads of our scientists. Lasers, chaos theory, electric cannons, future energy, green chemistry, smart clothing - these and other topics were presented during these discussions.

How much order is in chaos? How can chaos be controlled? Professor Kęstutis Pyragas, the FTMC physicist, one of the most well-known Lithuanian scientists, answered these questions in a program **WITHOUT MASKS** of radio station LRT KLASIKA. There is a well-known scientific term "Pyragas method" used in chaos theory, while the mathematical models of Pyragas are used for studies of Parkinson disease. In the program, K. Pyragas talks not only about chaos theory and why accurate future weather forecasts are impossible, but also remembers the beginning of his life in exile and his family, where the respect for science was an important issue.

What good could be done using lasers and what are the scientists doing with lasers these days? All this and much more was in the talk of Dr Lina Grinevičiūtė from FTMC Optical Coatings Laboratory, Department of Laser Technologies in the webcast **FANTASTIC COFFE-SHOP** of the fantasts society "Tolkien Lithuania".

How dangerous are the medicines generated by artificial intelligence and what is the credibility in science? Dr Linas Vilčiauskas, the Head of the Chemical Engineering and Technology Department, talked to news portal Lrytas.lt in its podcast **DI ID** devoted to artificial intelligence. The scientist leads the team of co-workers who designs, manufactures and develops new materials for various devices designed to store or convert energy from one form to another (for example, environmentally friendly sodium-ion batteries or turning water into hydrogen). According to L. Vilčiauskas, about 10-20 percent of his scientific activity today is related to artificial intelligence, and the real revolution in this field is just at the beginning.

Dr Mindaugas Karčiauskas, the FTMC researcher at the Department of Fundamental Research, talked about the latest progress in studies of gravitational waves in LRT program **GENE OF CURIOSITY**. The scientist, whose main field of interest lies in the very early Universe studies, gained his experience at CERN laboratory and recently returned to Lithuania from Lancaster University, UK.

Among numerous scientific experiments, the studies of fluorescencing molecules comprise an important part. Such experiments allow to study extremely small objects and are important in medicine, biology and other fields of science. These experiments are also performed by the scientists of the FTMC Plasmonics and Nanophotonics Laboratory, Department of Laser Technologies, who have discovered a method to prolong the fluorescence of such molecules up to tens of times. This research was presented by Dr Zigmas Balevičius, Dr Justina Anulytė and Dr Ernesta Bužavaitė-Vertelienė in the LRT TV program **GOOD MORNING, LITHUANIA.**

Why is it vitally important that the time in Lithuania would be precisely correlated with the global time? The FTMC physicist Dr Rimantas Miškinis, the Head of the Time and Frequency Standard Laboratory of the National Metrology Institute, talked about it to **LNK NEWS PROGRAM**. "The purpose of our laboratory is to support, maintain and manage the atomic clock system. Currently, we have two working atomic clocks that are connected to the global time formation system. There is no "one main clock" in the world, but there are about 600 atomic clocks" - said the scientist.

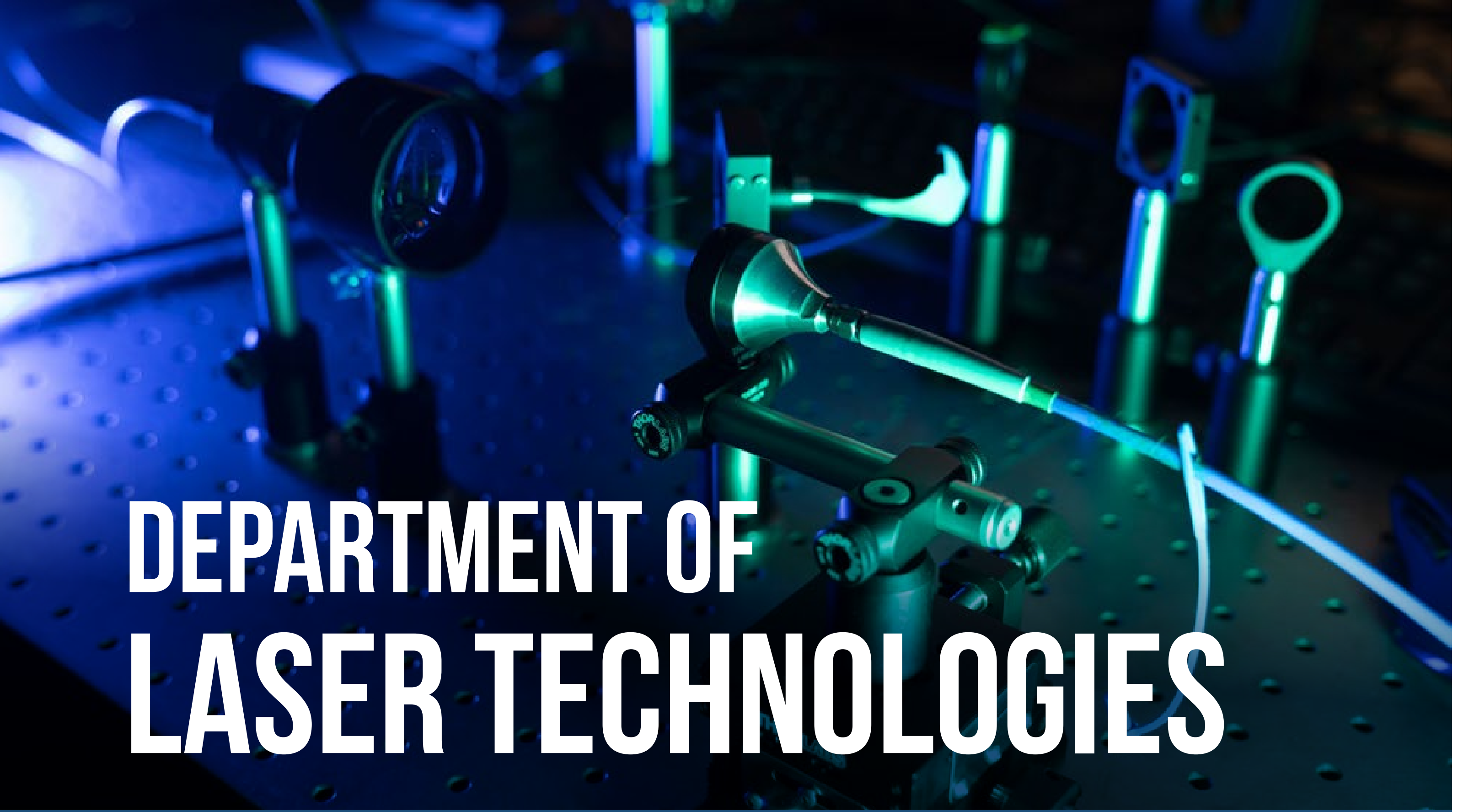
BEYOND SCIENCE

Something new happens every day in the FTMC, the largest scientific research center in the Baltic States, and the year 2024 was no exception. In addition to science-related events (articles, innovations, defended PhDs, scientific awards), the active, creative and youthful FTMC community organizes and participates in various extracurricular activities. These are just a few examples:

- All colleagues are kindly invited to become the members of FTMC Running Club. It's a no-obligation membership, all about having a good time, emotional and physical health, and small wins. The club organizes running holidays not only for FTMC employees, but also invites colleagues from Vilnius University and Vilnius Gediminas Technical University. Club members are active participants and winners of runs organized in Vilnius.
- The National Blood Center organizes blood donation campaigns at the FTMC, in which participate as our employees, as well as researchers and students from other institutions. We have colleagues who donate blood for the 20th or 30th time. It is simply an opportunity to help others.
- Mardi Gras, spring and autumn festivals, Christmas fair, all these events are usually organized by Janina Stankevič, the initiator of our "Leisure laboratories". These are the occasions when the colleagues share their own creations: ceramics, home fragrances, confectionery, handicrafts, jewellery, etc. Everyone is brought together by a cozy conversation over a cup of tea.
- The annual traditional FTMC Christmas quiz organized by Rusnė Ivaškevičiūtė-Povilauskienė, a researcher of the Optoelectronics Department, attracts an increasing number of teams not only from FTMC, but also from Vilnius University.
- Another tradition is the 5th FTMC chess tournament, where more and more participants test their wits and strength. Here we can meet as our scientists coming directly from the laboratories, as well as our guests from other institutions. During the tournament, there is no shortage of both great emotions and stress characteristic for every sports event.





DEPARTMENT OF LASER TECHNOLOGIES

"Light is essential for human live, and we employ lasers to make it easier and more comfortable"

Dr. Gediminas Račiukaitis
Head of Department, Principal Researcher
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The Department of Laser Technologies focuses its research on optics, lasers, laser technologies and additive manufacturing. Our researchers were active in their fields on structural all-silica coatings, lasers, plasmonics, laser processing, laser-assisted selective metal plating, and international events. The research results are illustrated in the next pages.

In addition, we were extremely active and successful in applying to Horizon Europe, CHIPS JU, the European Defence Fund, NATO, EuroStars, and Lithuania-Taiwan research projects. European Chips Act and defence initiatives open new opportunities.

SUINK – a Horizon project, we joined through the Hop-on scheme on sustainable electronics. New *LASER-PRO, ChipsC2-LT* and *EPACE* projects will be launched at the beginning of 2025. The H2020 project *PULSATE* was finished but we continue to support local companies in adopting laser technologies through the Digital Innovation Hub *EDIH.LT,* providing test-before-invest services. Laser-based advanced and additive manufacturing technologies are one of the key enablers of digital manufacturing.

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 within H2020 projects *Multiscan 3D* and *i.FAST* and user calls at the ELI – Extreme Light Infrastructure.

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. Well-established relations with partners from Germany, France, the UK, Australia, South Korea or Taiwan provide new research and knowledge transfer opportunities.

Efficient ablation, further GHz burst polishing, and surface texturing by ultrafast laser

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https://doi.org/10.1002/adem.202302262

The high-power ultrafast laser, capable of operating in various irradiation regimes (including single femtosecond pulses and GHz bursts), serves as a versatile tool for rapidly milling three-dimensional cavities and crafting functional surfaces on stainless steel. This single laser source enables efficient ablation, GHz burst polishing, and surface texturing with remarkable precision. These advancements pave the way for new industrial applications of ultrafast laser technologies.

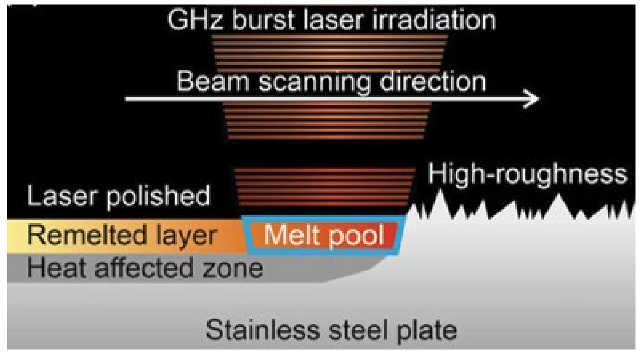

Fig. 1. Surface polishing process using GHz burst laser irradiation.

Bi-stability in femtosecond laser ablation by MHz bursts

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https://doi.org/10.1038/s41598-024-54928-7

This study demonstrates control over the bi-stable behaviour of laser ablation efficiency and quality through fluence and burst length. Plasma shielding of incoming laser radiation caused drops in ablation efficiency for every even-numbered pulse in the burst. A model of burst ablation efficiency was developed, incorporating plasma-induced attenuation, and a novel mathematical recurrence relation was derived to link the efficiency of consecutive pulses. The model predicts bi-stability and efficiency jumps based on burst pulse count and peak fluence, aligning well with experimental results. Optimizing the shielding effect with three-pulse bursts achieved exceptionally high laser ablation efficiency.

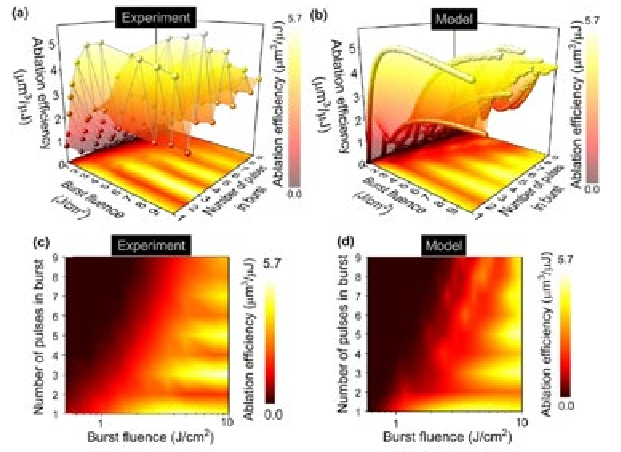

Fig. 2. Laser ablation efficiency of copper (colour scale) dependence on the burst fluence and the number of pulses in femtosecond burst: (a, b) 3D views and (c, d) 2D maps of experimental and modelling results.

Tuning SERS performance through the laser-induced morphology changes of gold nanostructures

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Differently shaped periodic gold nanostructures on the surface of a thin metal film are fabricated utilizing the direct laser writing technique. The variations in the energy of single femtosecond pulses lead to the formation of morphologically distinct hollow nanostructures. The arrays that excite hybridized plasmonic modes are characterized by electron microscopy and assessed for surface-enhanced Raman spectroscopy (SERS). Plasmonic properties are investigated through SERS using the adsorbed 4-mercaptobenzoic acid (4-MBA) molecules. The development of sharp tips in the nanostructures is initiated by the higher-energy laser pulses, while the structure formation principle itself is altered by the thickening of the film. The change in the structure shape and gold layer thickness tune the SERS signal and the enhancement factor (EF), leading to an EF of 10^7. Such a factor enables the future prospects of the arrays to be applied for single-molecule detection.

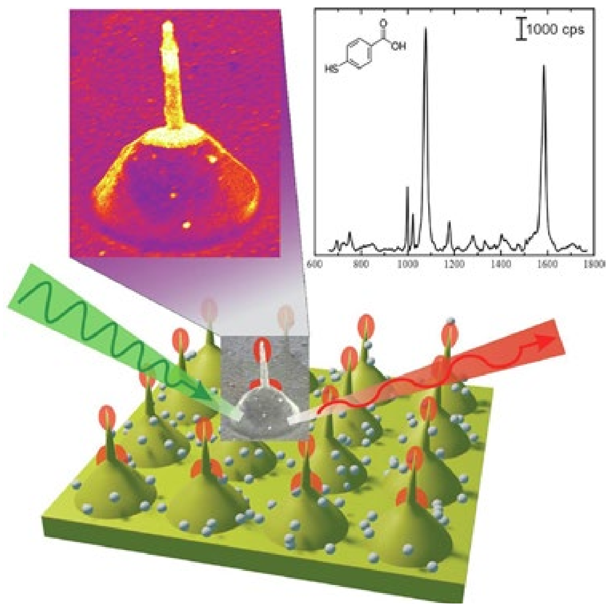

Fig. 3. Raman scattering spectrum obtained from the nanostructures on a 100 nm thick gold film and an illustration of the scattering from the grating with 4-MBA molecules.

Stainless steel colouring using burst and biburst mode ultrafast laser irradiation

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https://doi.org/10.1016/j.optlastec.2024.110561

Using a femtosecond pulse laser in various burst regimes, colours were successfully generated on stainless steel. The dependence of these micromachined colours on fluence and the number of pulses within burst regimes was investigated, with the resulting colours analysed and their origins explained. Demonstrating the flexibility of this method, intricate, multicoloured images were created with fine details. The surface structures responsible for the colours mimic natural phenomena and exhibit hydrophobic properties, significantly enhancing their potential applications.

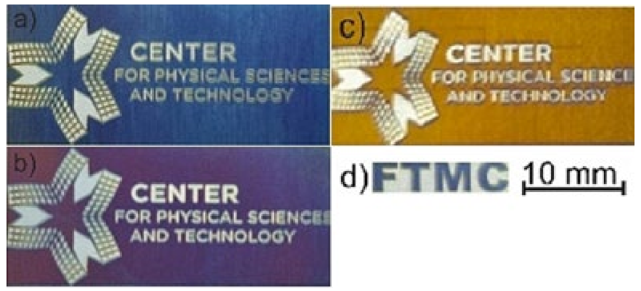

Fig. 4. Laser-coloured FTMC logo in various colours:
a) blue @ fluence 1.5 J/cm^2;
b) purple @ fluence 1.5 J/cm^2;
c) orange @ fluence 1.1 J/cm^2;
d) FTMC letters in blue colour @ fluence 1.5 J/cm^2.

Formation of highly tunable periodic plasmonic structures on gold films using direct laser writing

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DOI: 10.1002/adom.202400172

The direct laser writing method is a promising technique for the large-scale and cost-effective fabrication of periodic nanostructure arrays exciting hybrid lattice plasmons. This type of electromagnetic mode manifests a narrow and deep resonance peak with a high dispersion whose precise controllability is crucial for practical applications in photonic devices. The formation of differently shaped gold nanostructures using the direct laser writing method on Au layers of various thicknesses is presented. The resonance peak is demonstrated to be highly dependent on the shape of the structures in the array. Thus, its position in the spectra, as well as the quality, can be additionally modulated by changing the morphology. The shape of the structure and the resonance itself pertain not only to the laser pulse energy but also to the grating period. By taking advantage of the highly controllable plasmonic resonance, the fabricated gratings open up new opportunities for applications in sensing.

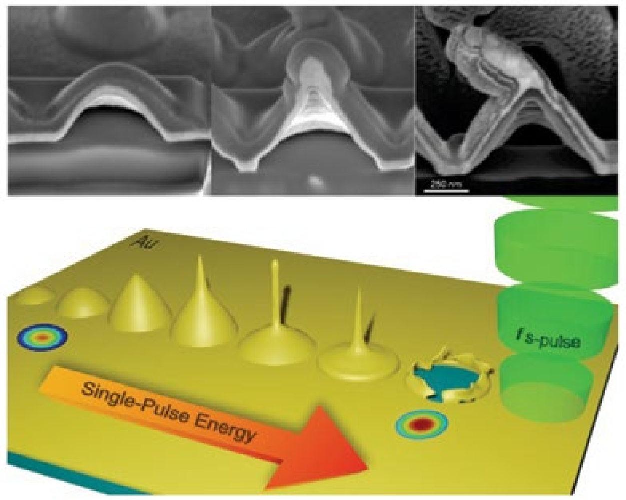

Fig. 5. (a) Cross-sections of bump, cone, and jet fabricated on 75 nm Au; (b) nanostructure shape dependence on pulse energy (50 nm Au layer).

High throughput and low surface roughness laser layer-by-layer milling using nanosecond (ns), picosecond (ps), and hybrid ns-ps pulses

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https://doi.org/10.1016/j.optlaseng.2024.108046

A comparative study of ablation efficiency and quality using conventional nanosecond (ns), conventional picosecond (ps), and novel hybrid ns-ps irradiation modes was conducted. 3D cavities milling in aluminium alloy CNC machined blank moulds was demonstrated and LED secondary optics moulds were fabricated using efficient laser milling at the picosecond regime and layer-by-layer slicing.

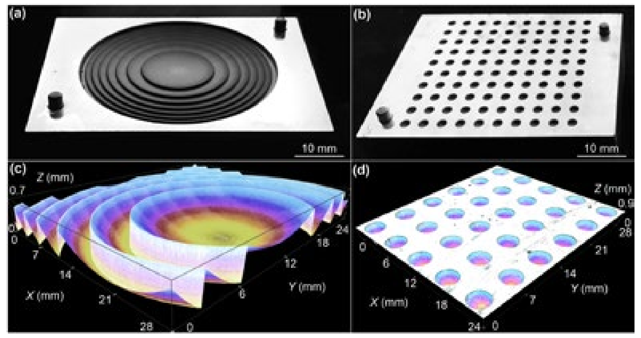

Fig. 6. Examples of efficient laser milling of aluminium moulds designed for LED diffusers. Digital camera images (a, b) and three-dimensional profiles (c, d) of a mould milled by picosecond laser.

A review on additive manufacturing of continuous carbon fibre-reinforced polymer composites using extrusion process

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Additive manufacturing (AM) is an advanced and sustainable manufacturing process to make functional parts from various materials. Fused deposition modelling (FDM) is the most widely used material extrusion (ME) additive manufacturing process to create composites using continuous fibre-reinforced polymer composites with improved mechanical properties and complex geometrical shapes compared to traditional manufacturing techniques. A thorough examination of the advancements and state-of-the-art developments in continuous carbon fibre (CCF) reinforced thermoplastic composite materials, focusing on their processing and fabrication through the ME method, is provided. The critical step is pre-impregnation of CCF before manufacturing, enhancing the mechanical properties of the composites. With varying printing process parameters, the mechanical performance of the produced composites could be altered. The review addresses the current technological challenges that limit the broader application of these advanced materials and proposes potential future directions for research and development.

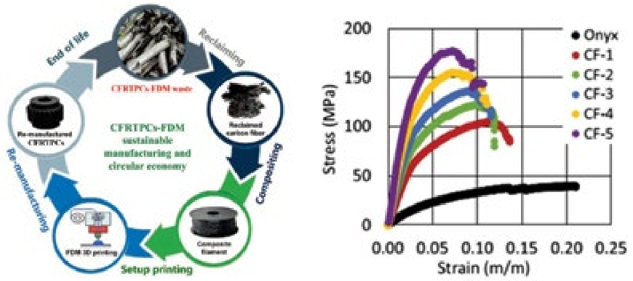

Fig. 7. The sustainable and circular economic manufacturing process of FDM and flexural stress-strain curves of Onyx and fiber-reinforced polymers.

Amplification of supercontinuum seed pulses at ~1078–1355 nm by cascade rotational SRS in compressed hydrogen

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https://doi.org/10.3390/app132413087

Higher order rotational Stokes combs covered the difficult-to-reach wavelength range from ~1.1 to 1.4 µm using broadband supercontinuum seed and circularly polarized pump pulses at high hydrogen pressure. The conversion efficiency of 52% was achieved with amplified pulse energies exceeding 3 mJ and the synthesized spectrum corresponding to ~14 fs pulses. The resulting pulses allow for a significant increase in image depth for nonlinear microscopy.

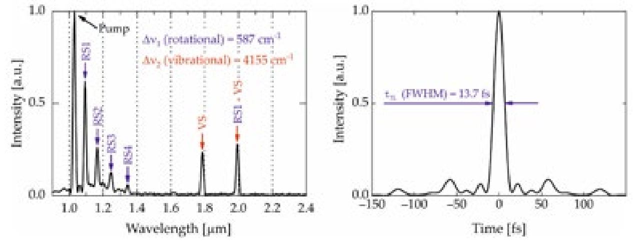

Fig. 8. Rotational Stokes comb spectrum (left) and transform-limited temporal shape (right).

Ultrafast 10 mJ, 100 W laser system featuring a directly laser-written depolarization compensation element

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Compared to other sophisticated active material geometries, the end-pumped geometry is much simpler and more efficient, but at power levels 100W and higher it suffers from thermal issues, such as thermal birefringence and bi-focusing. The article presents the application of a quite efficient technique – spatially variable retardation plate (SVRP) used to reduce depolarization losses and improve the spatial beam properties. SVRP was made using nano gratings inscription in the silica glass substrate (Fig. 9). Application of the experimental SVRP led to the reduction of the depolarization by a factor of two (Fig. 10). The laser system described in the article ran at 10kHz and generated high spatial quality laser pulses of 90W mean power of sub-picosecond duration. In the article, the modelling results, which show the way to modify SVRP for even better compensation performance, are presented.

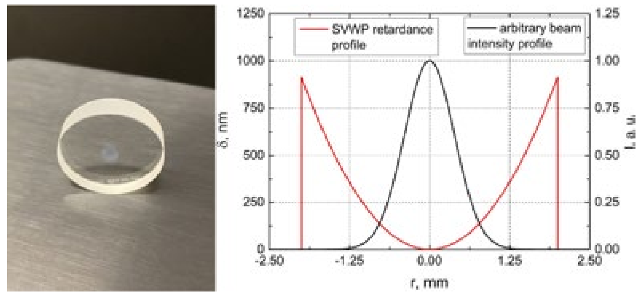
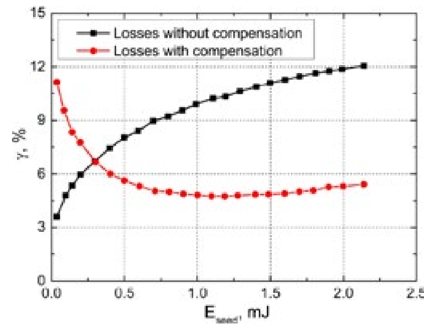


Fig. 9. Picture of a spatially variable wave plate and retardance profile of an SVRP plotted against the intensity profile of an arbitrary laser beam.

Fig. 10. The dependency of depolarized signal energy and depolarized signal fraction on seed pulse energy in the second amplifier stage. The total pump power was fixed at 290 W during the experiment.



Non-reciprocal optical phase shifter based on the Sagnac effect and its implementation as an optical isolator

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Most devices for non-reciprocal light transmission are based on the magneto-optical Faraday effect. Non-reciprocal light propagation can also be achieved using the Sagnac effect. It is particularly attractive as it does not rely on the optical properties of specific materials but arises from the fundamental properties of space-time itself. The proposed principle of optical isolator based on the Sagnac effect can be applied across the entire electromagnetic spectrum, from radio waves to X-rays.

We demonstrated a non-reciprocal phase shifter (NRPS) based on the Sagnac effect and provided examples of its use in the integration of various optical circuits. The scheme of a non-magnetic optical isolator with NRPS embedded in a Sagnac interferometer was experimentally demonstrated. A ratio of 110:1 in light transmittance between the forward and backward directions was obtained.

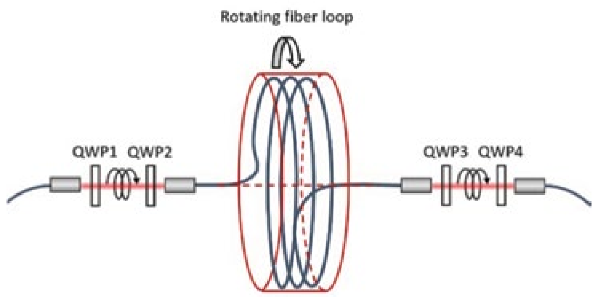

Fig. 11. Principal scheme of a non-reciprocal phase shifter.

Laser-machined two-stage nozzle optimised for laser wakefield acceleration

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https://doi.org/10.1017/S0022377824000059

Two-stage supersonic gas jet nozzles were modelled and manufactured, enabling the formation of adaptive plasma concentration profiles. The first 200–300 μm diameter nozzle stage is dedicated to 1 % N2 + He gas jet formation and electron injection. By varying the pressure between the first and second stages of the injectors, the electron injection location could be adjusted, ensuring the maximum acceleration distance. By varying the concentration of the nitrogen in the gas mixture, the charge of the accelerated electrons could be controlled. The second nozzle stage is designed for acceleration in fully ionised He or hydrogen gas and provides an optimal plasma concentration for bubble formation depending on the laser pulse energy, duration and focused beam diameter. The shock wave reflected from the straight section of the wall propagates parallel to the shock wave of the intersecting supersonic jets and ensures a minimal gap between the jets. The second-stage longitudinal plasma concentration profile could incorporate an increasing gas density gradient to compensate for dephasing between the electron bunch and the plasma wave due to wave shortening with increasing plasma concentration.

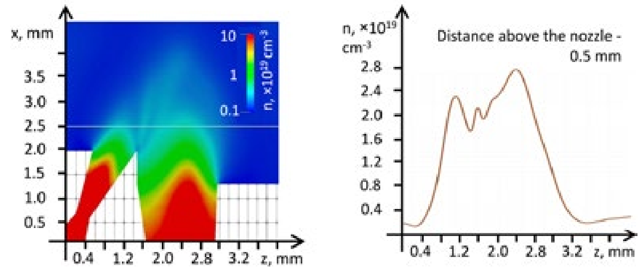

Fig. 12. (Left) Helium gas density diagram of the two-stage supersonic nozzle and (right) longitudinal gas concentration profile at the backing pressure of 27 bar along the laser propagation path at a 0.5 mm distance above the outlet of the injection stage of the nozzle simulated using the OpenFOAM CFD software.

Fig. 13. Image of the nozzle with two different gas supply systems assembled into 3D metal printed support.

Comparative analysis of microlens array formation in fused silica glass by laser: femtosecond versus picosecond pulses

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https://doi.org/10.1016/j.jsamd.2024.100804

Ablation using femtosecond pulses demonstrated a higher level of stability, ensuring more predictable optical element surface formation. In contrast, the use of picosecond pulses led to an increase in the thickness of removed material with each ablated layer. After 256 scans, the surface roughness S_a was about five times lower (0.52 μm) when femtosecond pulses were used. After CO_2 laser polishing, the surface roughness was reduced to <30 nm, which is suitable for optical applications and the microlens array was fabricated as a technology demonstrator.

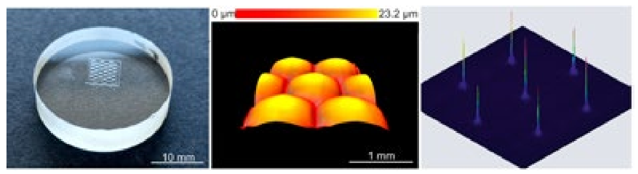

Fig. 14. Optical and topography images of a micro-lens array formed with femtosecond laser pulses together with an intensity image of the diode laser beam focused with micro-lenses.

Hybrid gold-silver nanoparticles synthesis on a glass substrate using a nanosecond laser-induced dewetting of thin bimetallic films and their application in SERS

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https://doi.org/10.1016/j.optlastec.2023.109956

The generation of hybrid gold-silver nanoparticles from different metal ratios by thermal heating thin metal films on a glass surface with a nanosecond pulsed laser is presented. The optical properties of obtained nanoparticles are dependent on localized surface plasmon resonance (LSPR), which can be tuned in the range of 400-530 nm by varying the ratio and order of the primary films. The various resonance widths suggest that different types of nanoparticles (monometallic or bimetallic alloy) with various concentrations and size distributions can be produced by laser-induced dewetting of thin bimetallic films. Substrates with engineered nanoparticles act as SERS substrates with a high enhancement factor (more than 10^5) using different excitation wavelengths (532 and 633 nm). Laser-based process for large-scale production of SERS substrates was demonstrated.

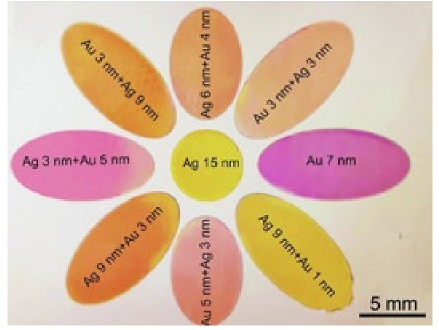

Fig. 15. Photograph of nano-particles on glass substrate obtained from Au, Ag, Au-Ag, and Ag-Au films of various thicknesses and ratios.

Fast and efficient bottom-up cutting of soda-lime glass using GHz bursts of short laser pulses

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https://doi.org/10.1016/j.optlaseng.2024.108490

In this work, we have investigated 4.8 mm thickness soda-lime glass cutting using the femtosecond laser GHz burst regime. To the best of our knowledge, we have shown the highest relative cutting speed and relative cutting efficiency compared to other studies on laser ablative cutting of glass. The highest cutting speed of 4.2 mm/s and linear cutting efficiency of 0.13 mm/J were achieved.

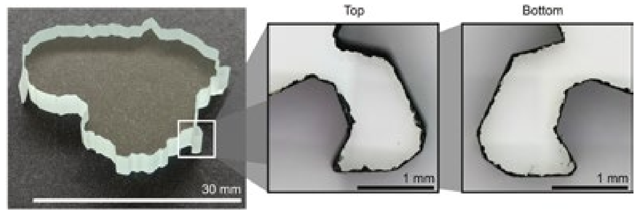

Fig. 16. Complex samples, cut with a bottom-up technique using a burst regime. Lithuanian borders, cut from 4.8 mm-thick glass with top and bottom surfaces inspected with an optical microscope.

Strongly coupled plasmon-exciton polaritons for photobleaching suppression

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https://doi.org/10.1515/nanoph-2024-0259

The fundamental understanding of coherent energy exchange via strong light-matter coupling between the plasmonic cavity and emitter opens new pathways in modification of chemical reaction rates, conceptually new types of nanolasers, Bose-Einstein condensation at room temperature, quantum optical nanodevices and advanced optical sensing. The influence of room temperature strong coupling between surface plasmon polaritons (SPP) and excitons on fluorescence lifetimes and photobleaching effects was investigated. The structure, comprising a thin metallic layer with an R6G dye layer, shows a clear shift in the SPP and R6G absorption lines, indicative of a strong coupling, with an evaluated Rabi splitting of 90 meV (Fig.17). Fluorescence lifetime imaging microscopy was then employed to assess photobleaching, revealing a significant 6-fold reduction in photobleaching effect in strongly coupled plasmonic-excitonic structures (Fig.18). Our findings indicate the pivotal role of strong light-matter interactions in reducing photobleaching effects and stabilizing fluorescence intensities, offering promising avenues for developing quantum multiparticle nanophotonic devices.

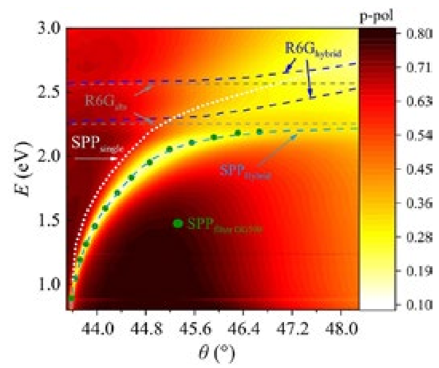


Fig. 17. The dispersion relations of strongly coupled polaritonic mode (green and blue dashed curves), single SPP (white dotted curve) and R6G excitons (grey dashed curve).

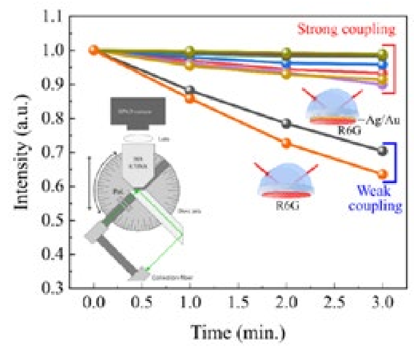
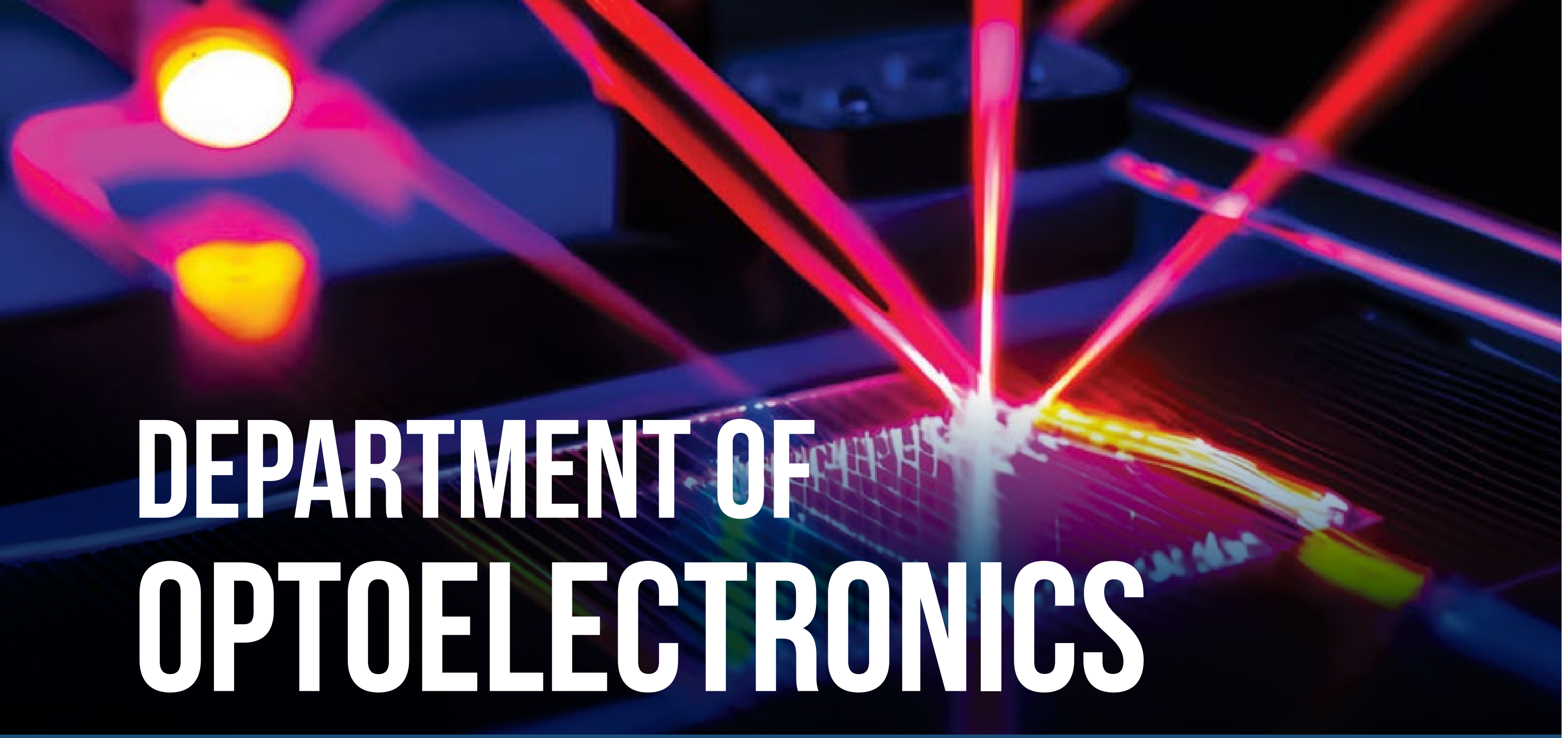


Fig 18. Photobleaching evolution in time of strongly coupled structure at various coupling strengths, and uncoupled or weakly coupled R6G dye layer.



DEPARTMENT OF OPTOELECTRONICS

"Continuing the tradition in optoelectronics and semiconductors, we promote balance between basic and applied research keeping inspiration to extend limits of knowledge, to enhance discovery impetus to go towards excellence… As Bertrand Russel says, "Science may set limits to knowledge, but should not set limits to imagination".

Prof. Dr. Gintaras Valušis

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The year 2024 displayed a large variety of activities in the Department – starting from internal seminars and exciting discussions in laboratories, efforts in preparing project applications, considerations on high-tech innovations and links with deep-tech companies – up to preparation of invited and contributed talks in international conferences and scientific publications in highly-ranked scientific journals. The Department organized two important international conferences – the *European Workshop on Innovative and Advanced Epitaxy (OPERA)*, closely related to the currently active COST network and traditional semiconductor physics-based conference *Advanced Properties and Processes in Optoelectronic Materials and Systems (APROPOS)*. The main research topics of the Department became more focused this year – it is dedicated to *semiconductor nanotechnologies for AIIIBV optoelectronics and terahertz-infrared photonics systems and devices*. We believe that semiconductor nanomaterials engineering and semiconductor-related research, as well as the development of high-frequency semiconductor chips and their hybrid/heterogenous integration, can be a basis for further progress in compact photonics and optoelectronics systems. Despite the dominating applied research-oriented profile, it is essential to keep strong attention to basic research to provide a prosperous source for generating new scientific knowledge. We gained versatile experience in semiconductor optoelectronics and terahertz research and have all the needed technological infrastructure based on molecular beam epitaxy (MBE), employing two apparatus by SVT and Veeco. The laboratories of the Department possess various experimental techniques spanning optical, terahertz and ultrafast methods, microwave and nanosecond electrical pulse-containing set-ups, and low-temperature facilities. Therefore, we are expecting further successful developments and promising results in compact terahertz imaging systems, 6G communication components and networks, GaAsBi- and antimonides-nanostructure-based optoelectronics, optical properties of semiconductor nanostructures, high-frequency GaN-nanostructure-based devices, and coherent optical tomography.

Currently, the Department consists of four Laboratories: Photonics Technologies and Devices, Semiconductor Optics, Terahertz Photonics, and Optoelectronics Systems Characterization. Last year marked a significant milestone as the Laboratory of Photonics Technologies and Devices established a new group dedicated to quantum technologies. Focusing on defects in wide bandgap semiconductors, the group aims to develop room-temperature spin-based qubits and single-photon sources for quantum sensing and communications. They launched two funded projects and a cross-departmental, internationally collaborative team of experts positioned to significantly impact the field. Led by Dr T. Paulauskas, head of the Lithuanian Quantum Technologies Association, the group is actively shaping the quantum technologies landscape to advance this field nationally and internationally.

Nonparaxial terahertz imaging using structured light engineered by silicon diffractive optics

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doi:10.1002/lpor.202301197

Principles of rational design and optimal assembly of non-paraxial THz imaging systems are established and exhaustively discussed. The research is focused on lens-less photonic systems composed solely of high-resistivity silicon-based nonparaxial elements, including the Fresnel zone plate, the Fibonacci lens, the Bessel axicon, and the Airy zone plate, all fabricated using laser ablation technology. The THz imaging systems were comprehensively examined via illumination engineering and scattered light collection from raster-scanned samples in a single-pixel detector scheme. The detailed evaluation of the imaging systems through the diverse metrics such as including contrast, resolution, depth of field, and focus, allow us to resolve promising tracks in the further evolution of compact and user-friendly THz imaging systems where sensors and optical elements are seamlessly integrated into a single chip.

Fig. 1. The published paper is featured on the front cover of Laser & Photonics Reviews.

Multifrequency digital terahertz holography within 1.39–4.25 THz range

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doi:10.1109/TTHZ.2024.3410670

The study demonstrates THz multifrequency digital holography across the range of 1.39 to 4.25 THz. It was shown that phase-shifting methods enable the qualitative reconstruction of multifrequency THz holograms combined into a single "coloured" image. This approach offers enhanced information about low-absorbing objects with improved quality, the information which can be achieved by eliminating unwanted artefacts associated with the dc term and the conjugate beam that forms a virtual image. The study reveals that THz holography can be used to investigate low-absorbing objects, as illustrated through the inspection of stacked graphene layers on a high-resistivity silicon substrate.

The results are published as an invited paper in a special IEEE Transactions on Terahertz Science and Technology issue dedicated to Selected Emerging Trends.

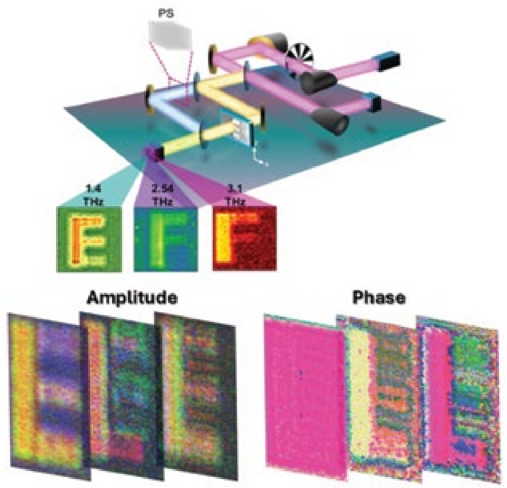

Fig. 2. Experimental set-up schematics (top panel) and amplitude and phase (bottom panel) distributions of the combined holographic images obtained at three different frequencies, 1.39, 2.52, and 3.11 THz.

Simultaneous transmission and reflection terahertz homodyne imaging system with integrated resonant C-shaped metalenses

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ACS Photonics (in press)

An advanced THz imaging system utilising a homodyne detection scheme integrated with polarising resonant C-shaped split-ring resonator (CSRR) metalenses is presented. Designed for a resonant frequency of 253 GHz, the system addresses the imaging challenges associated with low-absorbing dielectric materials. The system offers substantial improvements over conventional direct imaging techniques by enabling simultaneous imaging in both transmission and reflection geometries, thus enabling a comprehensive evaluation of relative absorption properties. Incorporating CSRR metalenses leads to a sub-wavelength resolution, significantly improving image contrast and providing more than double the dynamic range—68 dB for homodyne imaging compared to 30 dB for direct imaging.

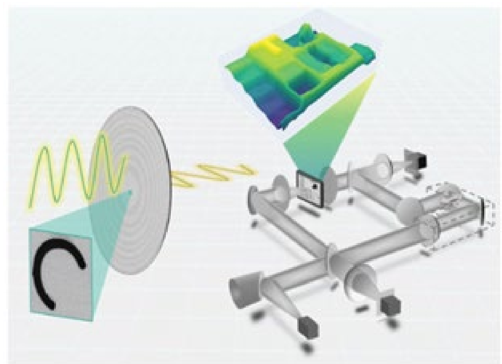

Fig. 3. THz imaging system, based on a homodyne detection scheme incorporating CSRR metalenses. The left-hand side features the CSRR metasurface which can rotate the polarisation of the THz beam. The imaging setup of the homodyne detection scheme is presented on the right. The upper inset depicts an example of THz homodyne imaging using metalenses recorded by combining six evenly spaced phase shift measurements.

The performance of the proposed imaging system is compared with THz time-domain spectroscopy, highlighting its advantages over conventional direct THz imaging techniques.

Internal quantum efficiency of GaAsBi MQW structure

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doi:10.1063/5.0234853

We present the first-ever emission efficiency calculations of GaAsBi/GaAs multiple quantum well structures. Internal quantum efficiency was determined by employing a new modified ABB* method, which improves the conventional ABC model by incorporating a trap-assisted Auger recombination channel. Our comprehensive study reveals that the ABC model significantly overestimates the internal quantum efficiency (21%) of bismides compared to actual measurements (0.01%). This new methodology not only enables reliable comparisons between structures grown and characterised in different laboratories but also provides quantitative insights into non-radiative recombination mechanisms. By establishing a more accurate efficiency measurement framework, our work addresses a critical barrier in optimising the low-temperature growth of GaAsBi structures for practical optoelectronic applications.

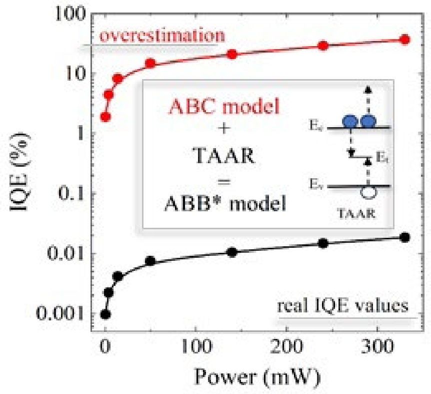

Fig. 4. Calculated emission efficiencies of GaAsBi/GaAs multiple quantum well structure employing the ABC and ABB* methods.

Photoconductive high voltage switch of Mn:GaN semiconductors

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https://doi.org/10.1109/TED.2024.3427098

A high-voltage switch involving sub-bandgap photo-excitation was developed for Mn-doped GaN semiconductors. Induced band tails of Mn were found to be photoconductive starting from the 700 nm wavelength threshold. Turn-on time of the switch was probed with short 10 ps duration laser pulses, revealing the voltage pulse duration and rise time values to be as short as 1 ns and 100 ps, respectively. The switch photoconductivity exhibited a 2 ns decay time at low-intensity laser pulses, while at the highest intensities, it increased up to 14 ns value. The resistance of the ON state can be regulated up to ten orders of magnitude under the change of the laser illumination intensity, which allows the switch to wire kilovolt voltage pulses on a load of 50 Ω impedance. The developed high-voltage switch with performance in a ns-time scale is beneficial for applications with high repetition rate operation.

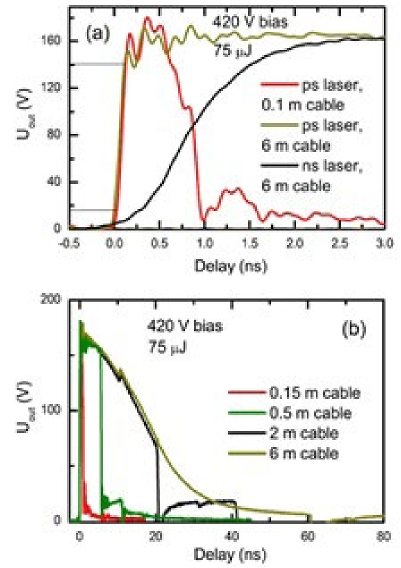

Fig. 5. Photoconductive signal decays at (a) short timescale window and (b) long timescale windows discharging different length cables under 420V bias voltage. The second peak at around 10 ns delay corresponds to an echo of laser excitation after the main pulse.

Broadband high-contrast-grating-type waveplates

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https://doi.org/10.1364/OE.521532

Waveplates and phase retarders are essential components to control the polarisation state and phase of the electromagnetic wave. The high-contrast-grating (HCG) waveplates utilising contrast between silicon (all-dielectric) and air refractive indexes were developed to perform as a quarter wave and a half wave plate in the THz frequency range. The waveplate possessed anti-reflective properties due to the specific inclination of the walls both in parallel and perpendicular directions to the grating axis, efficiently suppressing the reflection losses for both transverse magnetic (TM) and transverse electric (TE) polarisations. The concept was validated by measuring transmission amplitude and phase spectra in a broadband range of THz time-domain spectroscopy and vector-network-analysis systems. Indeed, the operation at other frequencies can be achieved by scaling the geometrical parameters. Such waveplates hold immense promise for applications in THz data communication, material spectroscopy, imaging, biomedical sensing, and scanning.

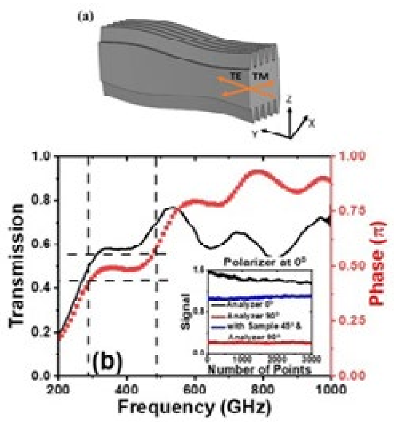

Fig. 6. (a) Design of HCG-type waveplate and its (b) transmission (left) and phase (right) characteristics across the frequencies up to 1 THz. Inset: signals at 400 GHz frequency in transmission mode with both polariser and analyser placed parallel (black curve), with both crossed (red curve) and with the HCG placed in between and oriented at 45 degrees (blue curve).

Microscopic description of a single-walled carbon nanotube film in the optical range

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https://doi.org/10.1103/PhysRevB.109.165409

Single-walled carbon nanotube (SWNT) films are promising materials to be used as transparent electrodes. Their optical response can be controlled by electrostatic doping. Despite the large amount of experimental data on the optical parameters of SWNT films, there is no theoretical approach for their satisfactory description. We propose to include additional terms in the existing quantum-mechanical model of SWNT conductivity that phenomenologically take into account the ultraviolet π plasmon and the contribution of σ electrons. The parameters of the additional terms are proposed to be determined from the experimental data obtained for the optical conductivity of graphene. This microscopic approach allows to describe the optical spectra of SWNT films. It predicts a strong suppression of the transverse response of SWNT due to the depolarisation effect. Also, the proposed approach satisfactorily describes the experiments obtained observing the azimuthal plasmon in SWNT films. The developed microscopic approach can be helpful in describing the optical parameters of SWNT films for various optoelectronic applications.

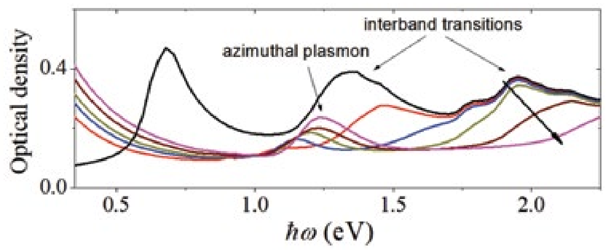

Fig. 7. The spectrum of optical density with clearly pronounced transitions in singled-walled carbon nanotubes.

Broadband terahertz photoconductive switches on centrosymmetric substrates

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Terahertz radiation spanning from 0.1 to 10 THz is critical in superconductors research, lattice vibration analysis, and various medical and biological applications, as many organic compounds exhibit characteristic absorption lines within this spectral range. However, working with terahertz frequencies requires specialised techniques that bridge the optical and electrical domains. One such technique, the photoconductive switches, has enabled us to capture a broad 0.1–7 THz bandwidth spectrum with a signal-to-noise ratio above 90 dB. This result was achieved by epitaxially growing an active semiconductor layer on a centrosymmetric substrate without polar phonons. Generally, photoconductive switch devices involve developing semiconductors with ultrafast photocurrents that decay within hundreds of femtoseconds, and the research is related to classical dipole antenna structures which allow the manipulation of radiation patterns. Although the THz waves hold significant importance for other scientific disciplines, today's photoswitches exhibit efficiencies below 1 %, requiring further technological advancements for decades.

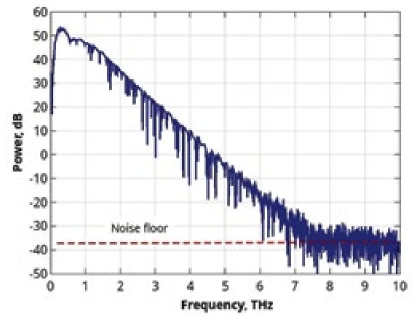

Fig. 8. THz spectrum, generated and detected with the photoconductive switches designed and fabricated by the Department of Optoelectronics.

Time-domain full-field optical coherence tomography with a digital defocus correction

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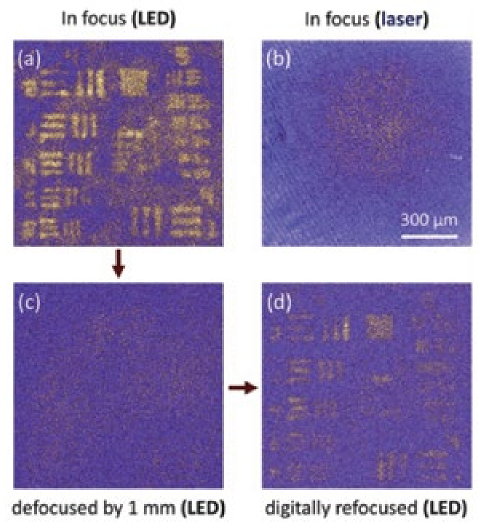
https://doi.org/10.1364/OL.520911

Full-field Optical Coherence Tomography (FF-OCT) provides deep-tissue, high-resolution 3D images of biomedical tissues using incoherent light, an interferometer, and a CMOS camera. While computational aberration correction is typically achieved in FF-OCT using spatially coherent laser sources, this study demonstrates that defocus correction is possible with an entirely spatially incoherent light source (white LED). Specifically, we show that sample defocus within a highly scattering medium can be digitally corrected over a wide defocus range by matching optical path lengths in the sample and reference arms and applying Fresnel propagation. We demonstrate successful digital defocus correction on both reflective and scattering samples, effectively compensating for up to 1 mm of defocus. Our approach yields a reduced speckle but with some signal loss compared to laser-based refocused FF-OCT images.



9. Digital defocus correction in FF-OCT imaging through highly scattering media: a demonstration using a USAF target beneath 400 µm of scattering material. (a) In-focus image of the USAF target. (b) The same image as in (a) but acquired with a laser. (c) USAF target image defocused by 1 mm. (d) Computationally refocused defocused USAF target.

DEPARTMENT OF ENVIRONMENTAL RESEARCH

"Our work is where science meets philosophy, a continuous conversation with nature to understand its language and hidden truths. Environmental challenges like air pollution and microplastic contamination aren't just technical problems to solve—they're a mirror, reflecting how our relationship with the Earth is evolving. As the Latin saying goes, 'Natura semper vincit'—'Nature always wins.' No matter how advanced our technology or how grand our ambitions, nature's laws remain the ultimate authority, reminding us that we must respect and adapt to the natural world rather than dominate it".

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The Department is dedicated to advancing research and developing innovative solutions to address environmental pollution challenges. By leveraging cutting-edge tools and methodologies, the team focuses on identifying the causes and mechanisms driving the impact of industrial activities and transport on environmental quality.

The Department is actively engaged in the following research and development activities: **Chemical composition, distribution, and sources of atmospheric aerosol particles:** research focuses on source apportionment and understanding the chemical composition and size distribution of aerosols, with implications for air quality management and climate system dynamics. Model-based investigations are applied to deepen the understanding of aerosol impacts, their properties and implications for air quality and regional and global climate systems. **Personal exposure to pollution in urban environments:** assessing exposure to particulate matter, black carbon, and ultrafine particles in urban settings to evaluate their potential health impacts. **Emerging contaminant removal technologies:** developing and exploring innovative solutions for removing contaminants in environmental and industrial applications, prioritising sustainable approaches to meet regulatory standards for complex mixtures in water, air, and soil. **Microplastic contamination in all environments and ecosystems:** The Department's research focuses on microplastic contamination across diverse environments and the human body, emphasising the investigation of their sources, spatial distribution, and ecological impacts, as well as evaluating the removal efficiency of technologies used in industry. The team uses an interdisciplinary approach to integrate citizen science-based monitoring programs to enhance data collection and foster community engagement.

MAIN ACHIEVEMENTS: Involvement in Horizon Europe EDIAQI project "Evidence-driven indoor air quality improvement" (grant agreement No. 101057497). EDIAQI aims to improve guidelines and awareness for advancing indoor air quality (IAQ) in Europe and beyond by allowing user-friendly access to information about indoor air pollution exposures, sources and related risk factors. The solution proposed by EDIAQI consists of characterising sources and routes of exposure and dispersion of chemical, biological, and emerging indoor air pollution in multiple cities in the EU. The project will deploy cost-effective/user-friendly monitoring solutions that will create new knowledge on sources, routes of exposure, and body burdens of indoor multipollutant.

Synergic use of in-situ and remote sensing techniques for comprehensive characterisation of aerosol optical and microphysical properties

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https://doi.org/10.1016/j.scitotenv.2023.167585

For the first time, a comprehensive set of ground-based and remote aerosol measurements was collected during an intensive summer field campaign in Vilnius in June 2022. The bivariate polar plots show the Conditional Probability Function (CPF) distribution of the probability of number concentrations higher than the 75th percentile. A distinction was made between nucleation (<25 nm), Aitken (25–100 nm) and accumulation (100–1000 nm) modes using the dataset of number concentration measurements by SMPS and APS (Fig. 1). The bivariate polar plots of particle number concentration (PNC) showed that the smallest (nucleation) particle mode was impacted by air masses from S and SE directions, which is consistent with the location of the city of Vilnius with respect to the position of the measurement station. In the case of the Aitken mode, there is no dominant direction. For the accumulation mode, the dominant direction of the air masses with high PNC is E and SE, which was also found to be dominant in the WPSCF or WCWT analysis of long-range transport.

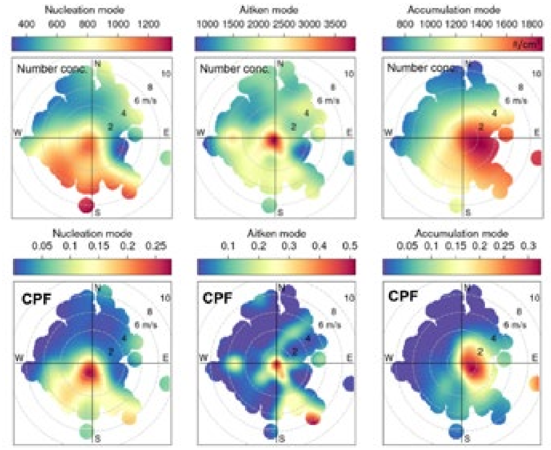

Fig. 1. Particle number concentration for June 2022: Bivariate polar plots for conditional probabilities of threshold overrun (75th percentile) for number concentration modes measured by SMPS and APS at the FTMC urban background station in June 2022.

Two distinct ship emission profiles for organic-sulfate source apportionment of PM in sulfur emission control areas

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https://doi.org/10.5194/acp-24-10815-2024

Factors and chemical components that belong to regional sources were combined and called Regional sources, which include the OOA, NO_3^-, NH_4^+, Cl^-, and regional sulfate subtracted from S-Ship. Note that an estimated 1% of PM_1 from the combined NO_3^-, NH_4^+, and Cl^- could be associated with low-S fuel emissions rather than Regional. However, there was enough uncertainty in this estimation that the 1% has been left associated with Regional. The heavy fuel oil (HFO) and low-S fuel contain the apportioned eBC, as explained above. Across the campaign, the source contributions to the measured PM1 were Regional (46%), Low-S Fuel ship emissions (14%), HFO ship emissions (12%), hydrocarbon-like organic aerosol (HOA) due to traffic or oil burning (10%), non-ship fuel eBC (9%), Peat (6%), and X-Ship emissions (2%). The Dublin Port ship-related factors comprised 28% (HFO, low-S Fuel, and X-Ship) of PM1, not counting ship traffic-related HOA and associated traffic eBC. It was difficult to attribute the HOA factor in Dublin Port to either ship-related traffic, city traffic, or oil burning for residential heating. Therefore, we estimate shipping-related emissions in Dublin Port contributed 28–47% of PM_1 (Fig. 2), as some significant portion of the HOA and traffic-related eBC was expected to also come from shipping-related activities such as ferry traffic, vehicles for moving containers, and crane engines.

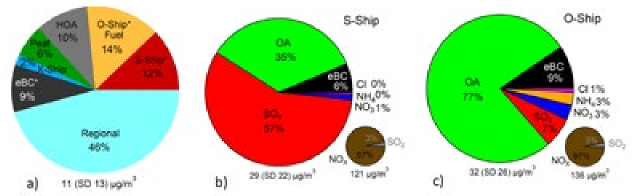

Fig. 2. Pie charts of the composition breakdown of the (a) source apportioned PM1 data, (b) S-Ship plumes breakdown of PM1 measured with gas data pie of SO_2 and NO_x, and (c) the same for O-Ship.

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

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

The presence of microplastics (MPs) in the human respiratory tract was demonstrated, i.e., fragments and fibres of MPs were detected. Our results showed that MP/NPs levels vary in the interval of 0.11–12.8 particles per 100 ml of bronchoalveolar fluid (BALF). The width of the particles varied from 20 μm to 283 μm, with an average of 49 μm. Similarly, the length of the particles exhibited variability, ranging from 35 μm to 1020 μm with an average of 203 μm. About 4.47% of microplastic particles were larger than 500 μm, and about 3.12% were larger than 300 μm. Via the optical analysis, most of the microplastic particles, i.e., 92.41%, were found in the size range of 10–300 μm. These results are consistent with the study that determined the size distribution of microplastic particles in indoor and outdoor air samples. The results showed that the vast majority of microplastic particles in the air were smaller than 100 μm (Fig. 3).

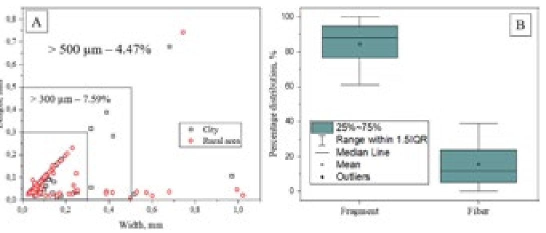

Fig. 3. (A) Size and (B) shape distribution of microplastic particles in BALF samples.

DEPARTMENT OF NUCLEAR RESEARCH

„We are a key link in ensuring excellence in applied nuclear research in Lithuania, from the safety of nuclear objects to the environmental aspects of isotope ratios."

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The activities of **the Department of Nuclear Research** include the development and application of conventional and innovative methods in the fields of nuclear fuel cycle technologies, experimental nuclear and mass spectroscopy, application of ion beam for the analysis and modification of material as well as the applications of lasers for the generation of ionising radiation.

The Experimental Nuclear Research Laboratory investigates the process related to ionising radiation and nuclear materials for safety of nuclear installations and new technologies for radioactive waste (RW) management: Ion beam methods for material analysis and modification are developed both for semiconductor materials and laser applications. Organic scintillator materials for detection and spectroscopy of ionizing radiation particles are investigated for RW monitoring application. The principles of the high energy particle acceleration are investigated using ultrashort laser pulses for practical application possibility in dielectric laser accelerator. Complementary information on material properties (magnetic properties, oxidation and corrosion of iron compounds) is determined by Mössbauer spectroscopy (combined with data of vibrating sample magnetometer for better characterisation of multiferroics).

In the Isotopic Research Laboratory, the special attention is paid to the environmental impact assessment of energy generating facilities, impacts of land-use change and crop rotation applications 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 (δ13C, δ15N, δ18O and δ34S) in environmental, archaeological and food samples stimulates new promising technologies.

Accelerator Mass Spectrometry Laboratory with 14C measurements ensures activities related to carbon dating and analysis of triple carbon ratio for dedicated samples.

The close collaboration of all laboratories allows the development of smart-environmental and environment-safe nuclear fuel cycle technologies as well as implementation of new analysis methods for public and business needs.

Dual carbon and sulphur isotopes as tracers of PM_1 pollution sources after COVID-19 confinement in Vilnius, Lithuania

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https://doi.org/10.1016/j.uclim.2024.101894

Particulate matter levels can change dramatically in an urban environment as the contribution of anthropogenic sources varies due to pollution reduction strategies and pandemic restrictions. Concentrations and isotopic compositions of sulphur and total carbon (TC) were measured for PM_1 (particles <1 μm) in size samples collected during the COVID-19 quarantine (2020-11-11–2021-03-16) in Vilnius, Lithuania. Dual carbon ($^{14}C/^{12}C$, $^{13}C/^{12}C$) and sulphur isotope analysis ($^{34}S/^{32}S$) was applied to quantify the contribution of fossil and non-fossil emissions to carbonaceous and sulphur containing PM1 (Fig. 1).

The contribution of fossil fuel sources was 1.3 times smaller compared to 2014–2015. The dominant sulphate sources were coal combustion (60 ± 10%) and biomass burning (40 ± 10%). Biomass burning becomes the predominant local source (up to 60%) in wintertime due to household heating activities.

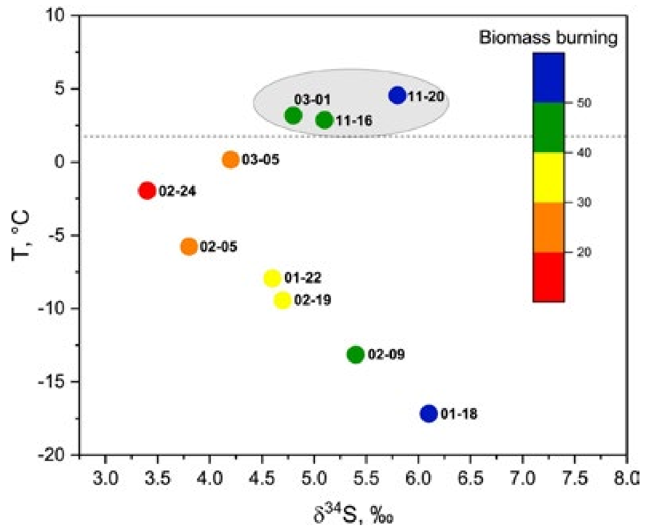

Fig. 1. δ34S dependence on average temperatures. Color gradient is used to represent the biomass burning fractions and sample dates are denoted.

Evaluating the impact of increased heavy oil consumption on urban pollution levels through isotope ($\delta^{13}C$, $\delta^{34}S$, ^{14}C)

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The impact of heavy fuel oil (HFO) consumption on urban pollution levels in Vilnius, Lithuania, was evaluated by examining the chemical and isotopic compositions of particulate matter and SO_2 gases during distinct heating periods. During the experiment, two heating periods were compared: one defined by the use of natural gas and biomass in local thermal power station (Fig. 2), referred to as the conventional heating (CH) period, and another one characterized by heavy fuel oil (HFO) usage. A significant increase in SO_2 and sulphate concentrations was observed during the HFO period and sulphate became the predominant water-soluble inorganic ion component in the particulate matter. In addition, stable isotope analysis of sulphur and elemental carbon (EC) revealed significant shifts in emission isotopic compositions, indicating altered source contributions and chemical processes affecting urban air quality during the HFO period (Fig. 3). However, radiocarbon analysis revealed a slightly decreased fraction of fossil-fuel combustion sources during the HFO period. The research underscores the potential of multiple stable ($\delta^{13}C$, $\delta^{34}S$) isotope and ^{14}C analysis as a powerful tool for tracing pollution sources in an urban environment.

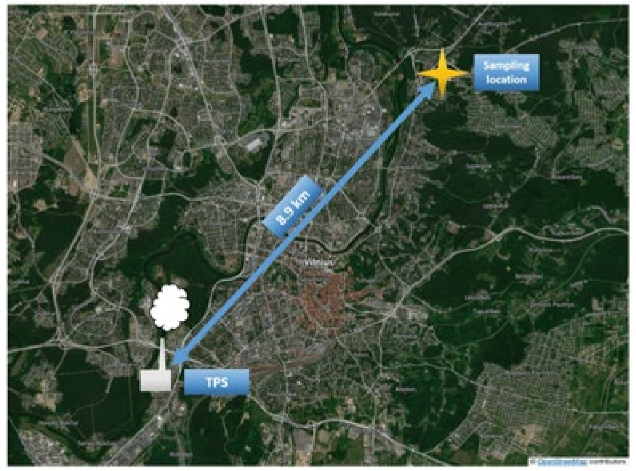

Fig. 2. Relative positions of the thermal power station and the sampling site (54.72 N, 25.32 E) in Vilnius

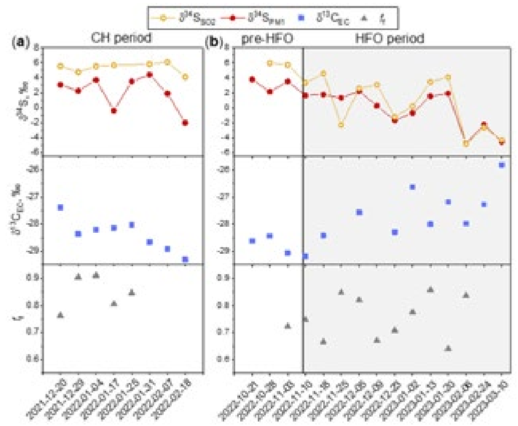

Fig. 3. Comparison of the heating seasons (a) 2021–2022 and (b) 2022–2023, displaying corresponding $\delta^{34}S$ values for SO_2 and PM_1 as well as $\delta^{13}C_{EC}$ and f_f values for PM_1. The gray shading indicates the period of HFO usage.

Optimisation of radioactive waste management technologies

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Completion of EU Horizon2020 EURAD and PREDIS, as well as the start of the new EURAD-2 project, which is a continuation of both previously executed projects, allows to gain and to use in practice the best world achievements in RWM technology and knowledge on RW predisposal and deep geological disposal management. In PREDIS the main FTMC activities have been focused on the nondestructive characterization of radioactive metallic waste (MRW). The applicability of several (HPGe, $CeBr_3$, NaI) detectors for discrimination of surface contamination/volume activity of MRW by comparing Compton-to-peak (C/P) ratios of real and simulated spectra (Fig. 4) has been evaluated. In EURAD, one of FTMC activities (CORI WP) was related to physico-chemical characteristics of cement superplasticizer based on Polymelamine Sulphonate which is used as admixtures ((super)plasticizing agents) in cementitious materials for radioactive waste immobilization in geological repositories. Portland cement (CEM I-type) was used in the leaching experiments (Fig. 5) including commercially available cement superplasticizer made from polymelamine sulphonate (PMS). Both the examination of the chemical and physical characteristics of CEM and the estimation of the long-term alkaline degradation of the PMS superplasticizer in various aqueous solutions by conducting spectroscopic analysis (using Raman and UV/Vis techniques) of the PMS hydrolytic solutions have been performed.

The outcome of the completed projects can be found at:
https://www.ejp-eurad.eu/publications
https://predis-h2020.eu/publications-and-reports/

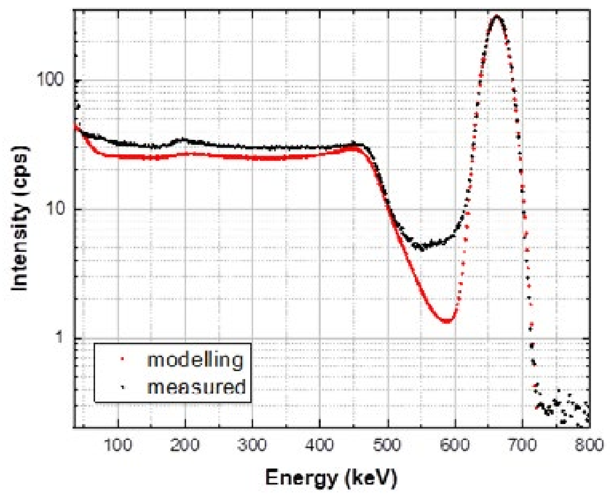

Fig. 4. Inter-comparison of γ-spectra of ^{137}Cs acquired by the $CeBr_3$ detector and modelled in case of point source on the surface of metallic reactor component.

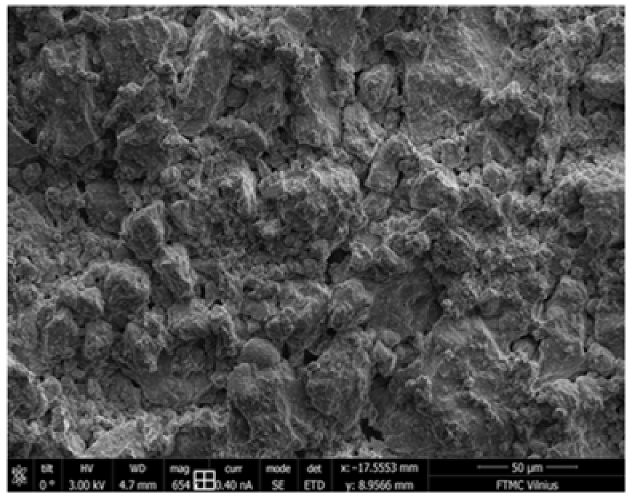

Fig. 5. SEM pictures of cement CEM I 42.5R sample before leaching (650 magnification).

Mössbauer study of reduction of ferric chloride in yeast growth media, by sugars and aluminum

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Iron compounds can be used in antimicrobial applications by exploiting the toxicity of divalent iron to living organisms due to the Fenton reaction. The Mössbauer spectroscopy was used to identify valence state of iron in the yeast growth media supplemented with ferric chloride and ferrous sulphate which show the growth inhibitory effects on tested *Metschnikowia* spp. and *Saccharomyces cerevisiae* yeast cells. High amount of Fe^{2+} was observed in the yeast growth media supplemented with ferric chloride as well as in the mixtures of ferric chloride with sugars indicating that Fe^{2+} is due to iron reduction by sugars. Mössbauer spectra shows even metallic iron α-Fe, valence state Fe^0, when the mixture of ferric chloride and fructose was placed on the surface of aluminum. This observation indicates that Fe^{3+} is reduced to metallic iron due to the cooperative reactions of ferric chloride with fructose and aluminum (Fig. 6). As ferric chloride can remove the surface oxide layer on aluminum, the reaction of water with aluminum releases hydrogen which participates in the reduction to metallic Fe. The relative amount of Fe^{3+} reduced to Fe^0 reached 68%.

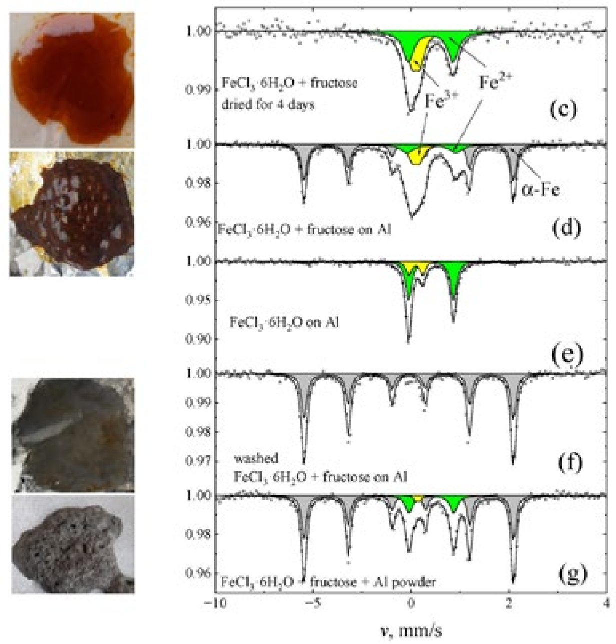

Fig. 6 (Right) Mössbauer spectra of samples shown on the left indicating the reduction of ferric chloride with fructose and aluminum. Yellow is Fe^{3+}, green is Fe^{2+}, and grey is α-Fe.

C and N stable isotopic composition analysis helps to investigate Blue Carbon storage and nutrients in the 2,000-year record of eelgrass (Zostera marina L.) colonization

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The historical colonization of eelgrass (Zostera marina) is an important marine vascular plant in cold-temperate coastal regions. Sediment cores from eelgrass meadows on the Swedish west coast dating back as far as 14,000 years were examined to understand the time course of eelgrass colonization and the subsequent modification of the environment. Sediment chronology and biogeochemical analysis (for C and N contents and $\delta^{13}C$ and $\delta^{15}N$ composition, lipid analysis, magnetic susceptibility (MS), XRF measurements to obtain elemental profiles) were used in statistical R (v. 4.2.2) analysis. It was found, that eelgrass colonization began approximately 2,000 years ago, coinciding with the development of shallow, sheltered conditions favoring eelgrass growth. As eelgrass became established, this led to substantial habitat and sediment changes, including a 20- and 24-fold increase in carbon and nitrogen accumulation, respectively. This highlights the crucial role of eelgrass as a provider of important ecosystem services, such as climate regulation, nutrient retention, and sediment protection. Also, the potential effects of climate change were examined on eelgrass growth and health, predicting that decreased water clarity and altered water flow pose the greatest risks. This study adds valuable insights into the relationship between eelgrass and its environment, aiding in conservation and restoration efforts to mitigate climate change and maintain essential ecosystem services. It emphasizes the importance of specific environmental conditions for successful eelgrass colonization and restoration (Fig. 7).

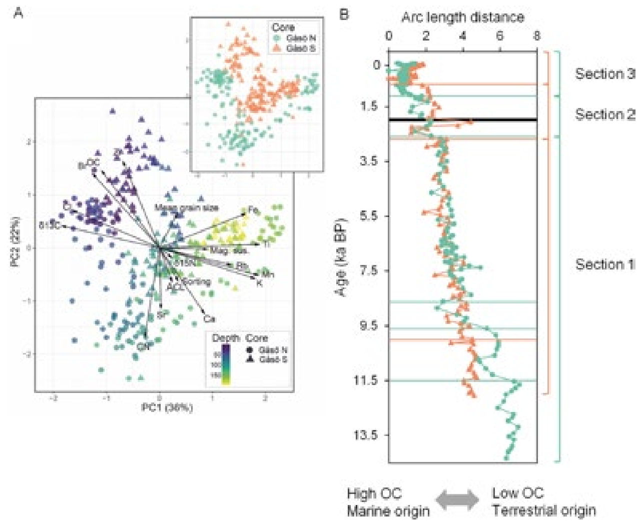

Fig. 7. Changes in sediment characteristics. The black line in panel (B) indicates the first appearance of seagrass-derived sediment in the paleorecord. Section 1 shows the time frame before seagrass establishment (as a baseline). Section 2 presents the period around seagrass colonization and Section 3 presents the seagrass stabilization phase

DEPARTMENT OF PHYSICAL TECHNOLOGIES

„Targeted manufacturing technology can make a new sophisticated idea work in practice. This is the main stimulus for us to look for new ways to use semiconductors with advanced properties for innovative practical devices“

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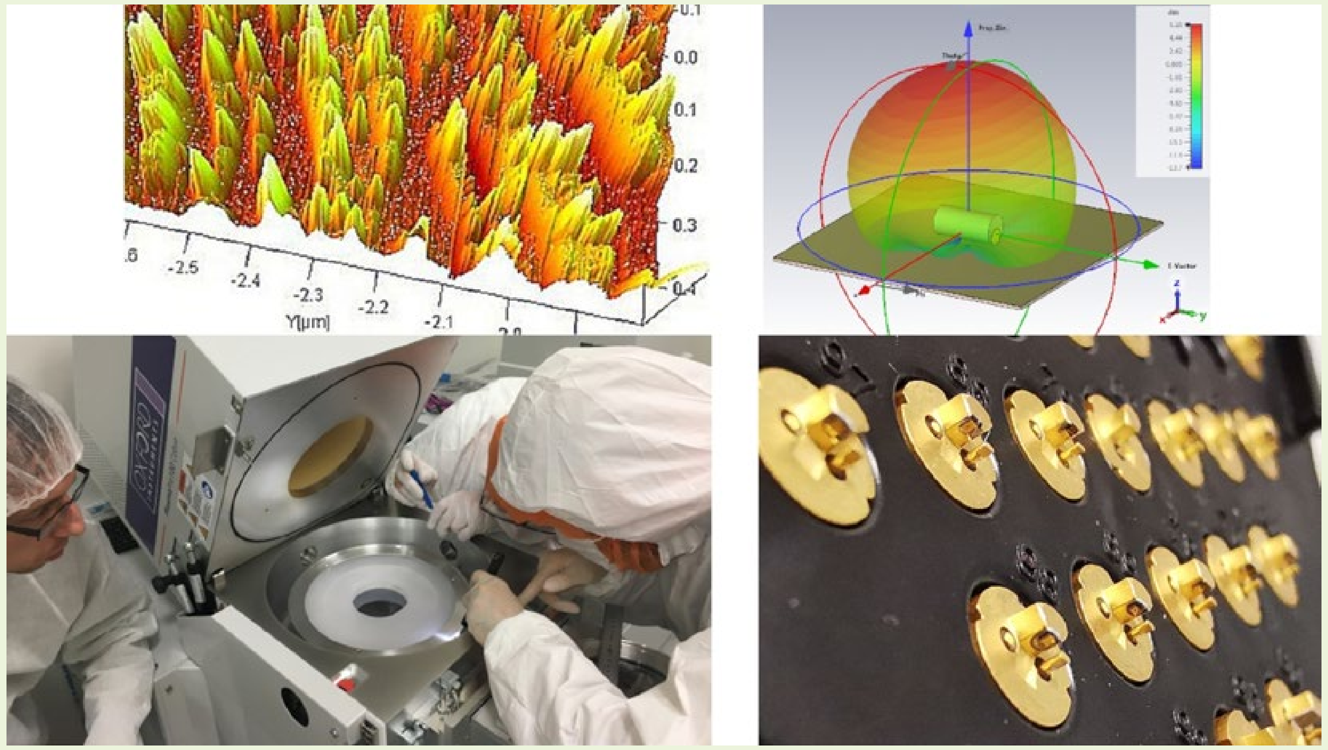
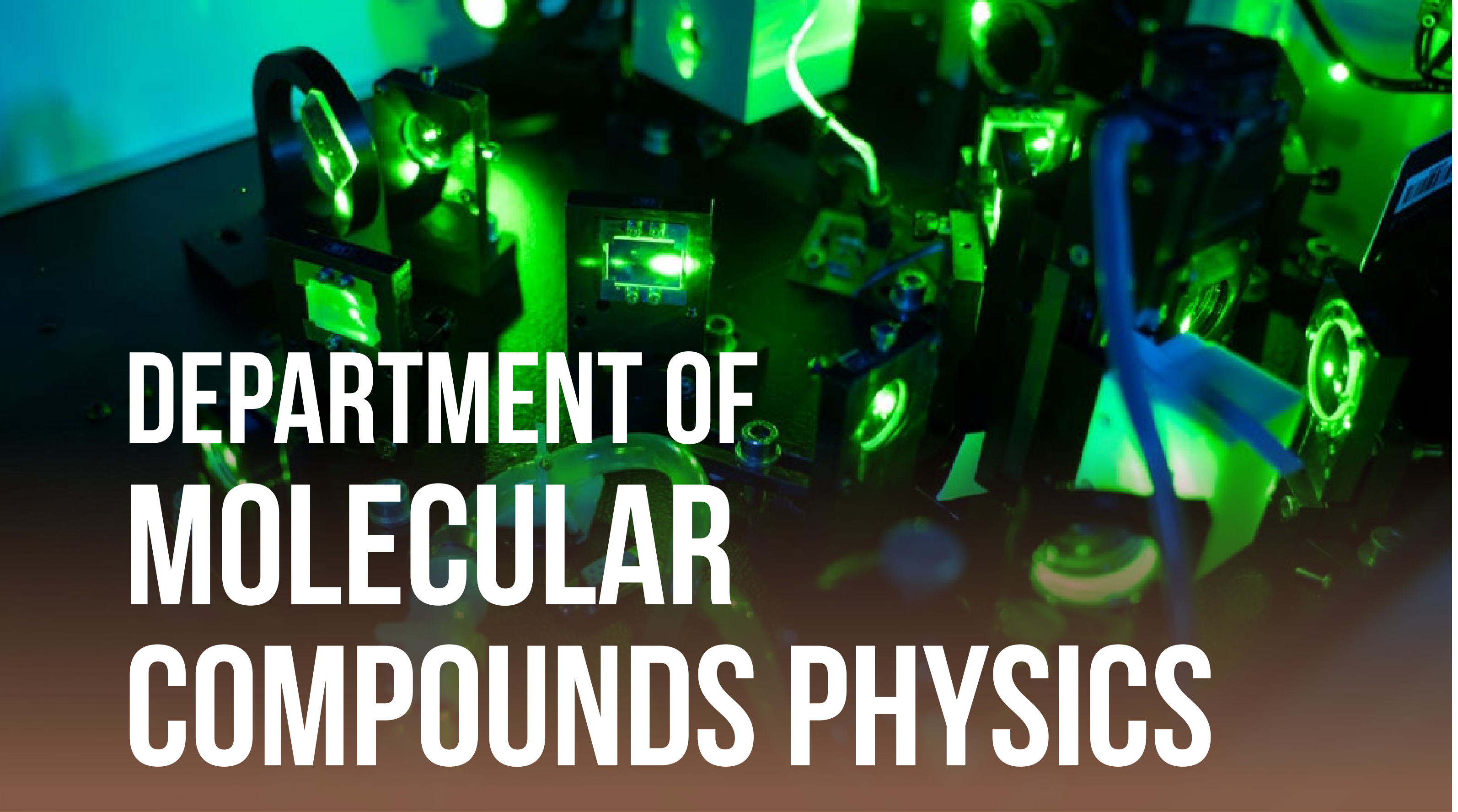
Investigations of the model structures and device prototypes combined with technology studies are acceptable to unlock the most effective ways to develop complex functional systems fusing the advanced electronic, electrical, and optical properties of semiconductors. The main topics of our research and development (R&D) are:

- **THE LOW-DIMENSION MATERIALS AND TECHNOLOGIES.** Multilayered structures with layer thicknesses reduced down to nanometres and even atomic scale opened access to unique properties of two-dimensional (2D) materials. Nano-crystalline graphene and transition metal dichalcogenides (TMDs), including molybdenum, titanium, and palladium disulphides, were investigated, aiming to intentionally create specific characteristics by the technologies, compatible with the CMOS processes. Perpendicular to the substrate arrangement of the graphene, nano-flakes were formed on silicon, as illustrated in the picture (top left). Specific optical characteristics were demonstrated for these structures. When the flakes were parallelly aligned with the substrate, the local bridges were proved to be opened by a compressing force for an electron flow across an insulating graphene sheet. Our recent studies also demonstrated unexpected electronic and optical properties in the 2D-TMDs-based structures.
- **MODEL DEVICES BASED ON NEW MATERIALS.** We combine classical three-dimensional (3D) semiconductors and the 2D-materials in the models. New concepts based on the van der Waals 3D- and 2D- combined structures were successfully proved, leading to an original PV-effect driven light detector with comparatively high (about 210 V/W) sensitivity to the illumination in the wavelength range of 500 – 1100 nm. Compatibility with integrated planar photonics systems is the most attractive aspect of novel model constructions, justifying our deeper research and development projects. Diverse constructions based on 2D/2D and 2D/3D are under investigation, aiming to develop the most acceptable design for both the broadband and the selected line detection of light in the near and mid-infrared intervals.
- **INTERACTION BETWEEN ELECTROMAGNETIC WAVES AND THE TARGETS.** Understanding electromagnetic radiation interaction with materials makes it possible to develop reliable approaches for practical problem solutions. Our studies are mainly focused on microwave and infrared (IR) radiation. A new type of dielectric antenna (top right in the picture) was proposed to detect the microwaves and harvest their energy. Interception and analysis of radar signals is the main task of the dedicated project, aiming to create a system capable of detecting and identifying nearby ships. The investigation of interactions between infrared light and materials aims to build a fundamental basis for the development of semiconductor laser systems for the distinction of specific chemical and physical features of selected targets.
- **PROTOTYPING OF THE DEVICES FOR PRACTICAL APPLICATIONS.** High-tech multi-component systems combining hybrid and monolithic integration of the elements are the primary targets in these investigations. Modern Clean Room technology infrastructure is used for it (bottom left in the picture). Our prototype system based on the IR semiconductors lasers (bottom right in the picture) was proven for in-line non-destructive quality control of polymer coating in project 01.2.2-CPVA-K-703-03-0019. The conversion of the features of processes and things into output data (IoT information creating nodes) is the main driving force behind our R&D on semiconducting nanostructures.

Based on the results of our investigations, five PhD theses were successfully accomplished over the last few years.





DEPARTMENT OF MOLECULAR COMPOUNDS PHYSICS

„We send photons to explore the life of molecules."

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The Department of Molecular Compound Physics focuses on the photoinduced electronic processes in natural and artificial molecular systems. Among them are biological photosynthetic and protein–DNA complexes, molecular aggregates, organic and perovskite solar cells, perovskite light-emitting diodes, perovskite-based light frequency down-converters, and other photonic materials and nanostructures that are important for optical and medical applications. The main tools of our work are time-resolved spectroscopic techniques, mostly fluorescence and ultrafast transient absorption. They are often used in combination with steady-state optical spectroscopy, optical microscopy and photoelectric measurements. Additionally, our department makes heavy use of modern non-linear microscopy techniques, such as CARS to reveal the distribution of distinct molecular species in various samples, SHG for research into cancer cells, or SMM to study fluorescing properties of single molecules that are unobservable in typical ensemble measurements. These advanced experimental techniques are supplemented with sophisticated data processing methods and rigorous theoretical modelling.

The goal of our fundamental research is to obtain a better understanding of electronic states and processes in various photoexcited materials. These include the evolution of excited states, their properties in excitonically coupled systems, charge transfer states in photosynthetic systems, the photogeneration of charge carriers, their motion, trapping, recombination and related processes.

Machine learning-enabled diagnostics of capsular invasion in thyroid nodules with wide-field second harmonic generation microscopy

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https://doi.10.1016/j.compmedimag.2024.102440

Custom-built wide-field second harmonic generation (SHG) microscope was used to investigate the morphology of the collagen capsule of papillary thyroid carcinoma (PTC). The detection of capsular invasion, where cancer cells breach the protective barrier, is crucial for the diagnosis and the correct choice of treatment. The acquired images of sections of whole PTC nodules (Fig. 1) were processed using texture analysis. The obtained dataset of intensity and texture parameters was analysed using machine learning (ML) methods. We were able to show that the collagen capsules in all analysed tissue sections were highly heterogeneous and exhibited different segments described by characteristic groups of features. This allowed to identify suspicious capsule areas, and microinvasions initially overlooked by the pathologist.

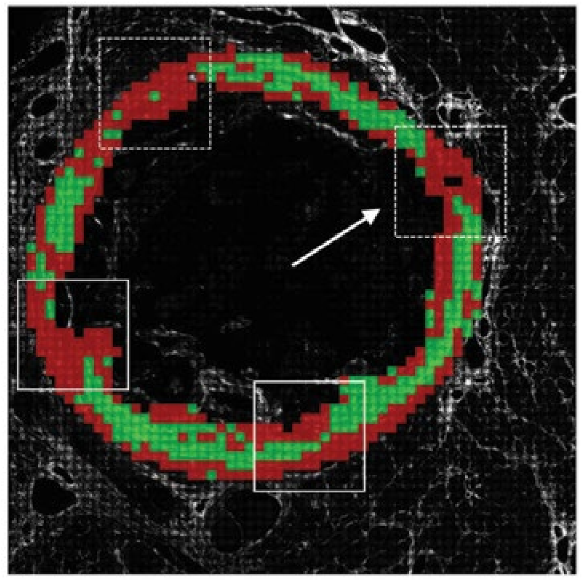

Fig. 1. SHG image with cluster maps of a section of a whole thyroid nodule. Solid rectangles denote invasions (annotated by pathologist), and dotted rectangles - suspect areas. Microinvasion is pointed out by an arrow.

Functional organization of 3D plant thylakoid membranes as seen by high resolution microscopy

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In the field of photosynthesis, only a limited number of approaches of super-resolution fluorescence microscopy can be used to probe the architecture of the thylakoid membrane in chloroplasts. We have used a custom-built fluorescence microscopy method called Single Pixel Reconstruction Imaging (SPiRI) that yields a 1.4 gain in lateral and axial resolution relative to confocal fluorescence microscopy and obtained 2D images and 3D-reconstructed volumes of isolated chloroplasts from pea *(Pisum sativum)*, spinach *(Spinacia oleracea)* and *Arabidopsis thaliana*. We show the complete network of the thylakoid membrane in intact, non-chemically-fixed chloroplasts at high resolution, from which the intensity of stromal connections between each granum can be determined.

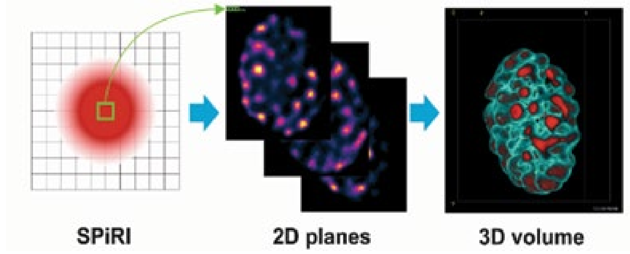

Fig. 2. A home-made microscope - Single Pixel Reconstruction Imaging (SPiRI) - was used to obtain 2D images (middle) and 3D-reconstucted volumes of intact plant chloroplasts to visualize entire thylakoid network (right).

Polarization nonlinear microscopy of diamond needles

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https://doi.org/10.1063/5.0202820

Polarization sensitive nonlinear optical microscopy technique was used to assess crystallinity of diamond microneedles. Strong signal in the vicinity of 1332 cm-1 Raman peak of diamond was utilized to get the CARS-image over the needle length and it demonstrated that the cubic lattice of diamond remains the same at both the micron-sized base and the nanoscale thin apex of the needle confirming its single-crystal nature. The results of the polarization-sensitive CARS measurements were described in terms of the third-order nonlinear susceptibility of diamond.

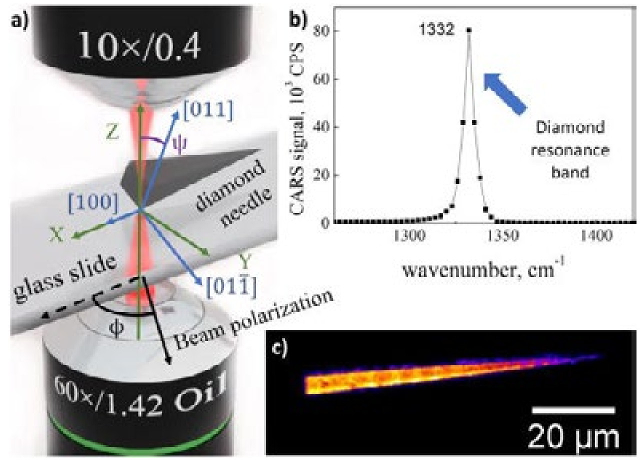
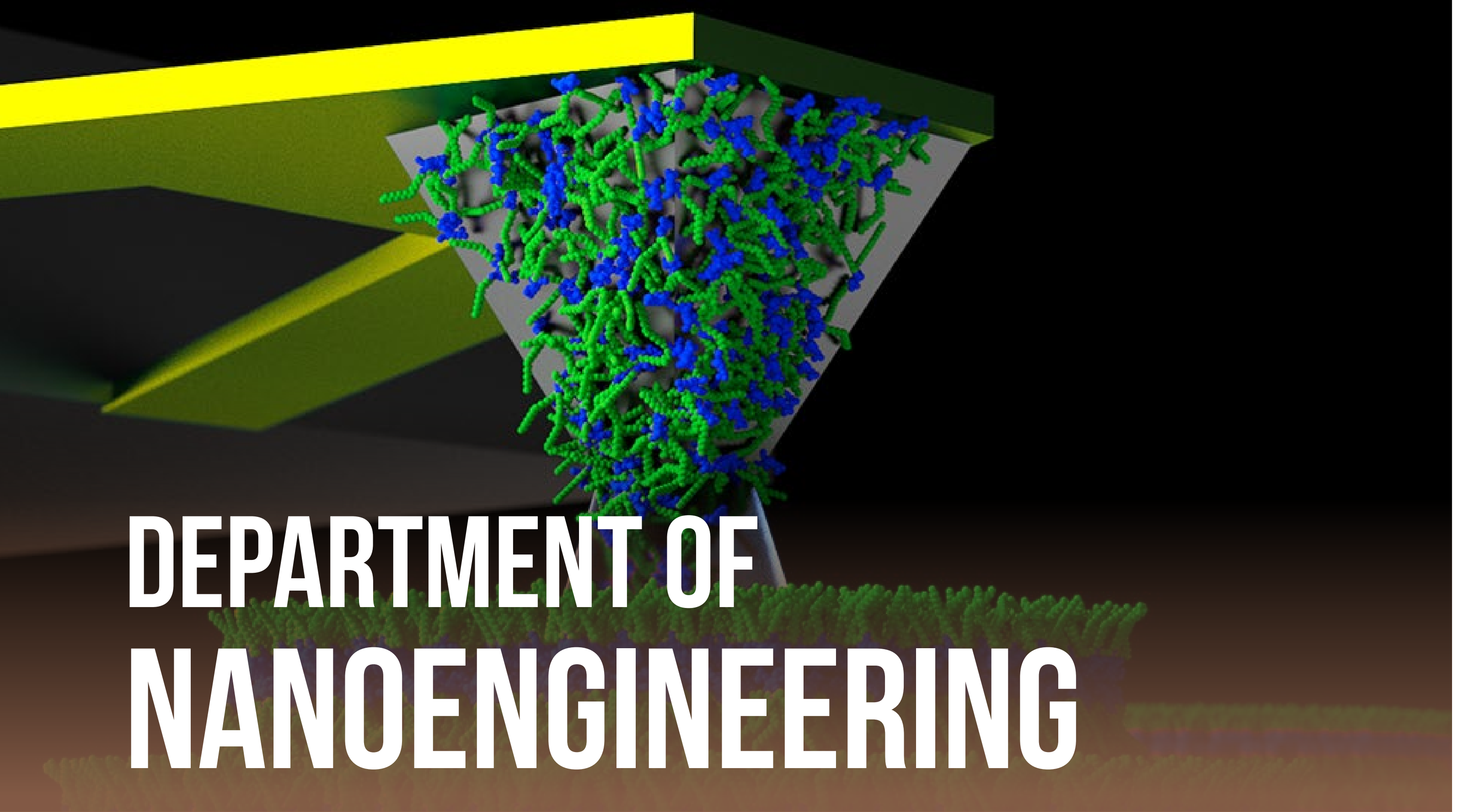


Fig. 3. (a) The CARS microscope setup and (b) the CARS-image of a diamond needle. CARS response depends on the orientation of the polarization azimuth of the collinear pump and Stokes beams. (c) Polarization measurements which prove single-crystal nature of a needle.



DEPARTMENT OF NANOENGINEERING

„We aim at understanding and employing the nanoscale phenomena at the interface of physical, chemical and living systems“

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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.

Bismarck brown assisted hydrothermal synthesis of nitrogen-modified reduced graphene oxide for selective electrochemical detection of dopamine

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https://doi.org/10.1016/j.surfin.2024.104041

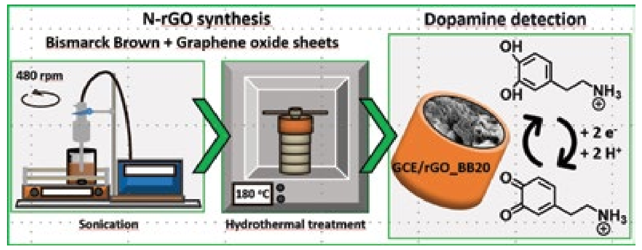

Fig. 1. A schematic representation of the BB application for the development of an electrochemical biosensor for dopamine.

Organic dyes can be used for functionalisation of carbon nanomaterials. Metal-free N-modified reduced graphene oxide (N-rGO) samples were prepared by convenient and cost-effective hydrothermal treatment of GO using two different concentrations of Bismarck Brown (BB), namely 20 wt.% and 50 wt.%. Structural characterization using XPS demonstrated that N content was 3.8 at.% and 10.6 at.% in the samples with 20 wt.% and 50 wt.% of BB, respectively. Due to N incorporation, interrupted carbon lattices and higher defective degrees were found by Raman spectroscopy in both samples. Noteworthy, that the sample with the lower BB amount exhibited a higher concentration of quaternary N species, a larger specific surface area and a higher electrical conductivity compared to the sample with higher BB amount. This led to superior electrochemical performance of the lower BB sample, demonstrating a LOD of 45 nM and sensitivity of 0.61 μA μM^{-1} cm^{-2} in a linear range of 0–15 μM. The proposed sensor displayed exceptional selectivity, reproducibility, repeatability and stability.

Investigation of picosecond laser-induced graphene for dopamine sensing: influence of laser wavelength on structural and electrochemical performance

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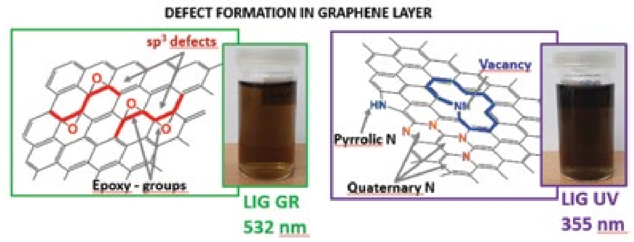

Fig. 2. Defects introduced to graphene by laser irradiation of different wavelengths.

Lately, laser-induced graphene (LIG) is gaining broader interest in electroanalysts community. In this research, LIG is employed to a straightforward synthesis using green (532 nm) and UV (355 nm) picosecond laser irradiation of graphene oxide dispersion. Structural analysis revealed that the laser operating at 355 nm is more favourable to producing material with a higher amount of the restored sp^2 network, larger graphene in-plane crystallite size, more abundant concentration of pyrrolic nitrogen and larger values of the optical bandgap. Contrarily, the 532 nm laser yielded with more abundant concentrations of epoxy groups, sp^3 defects and amorphous carbon. Electrochemical detection of dopamine exhibited potential for both samples as electrode substrate material. Nevertheless, the analytical parameters of the sample treated with the 355 nm laser surpass those of the 532 nm laser. The most probable reason is the enhanced electrochemical activity due to presence of pyrrolic N and vacancies in the structure of the sample treated with the 355 nm laser.

Interfacial structure and protein incorporation in sparsely tethered phospholipid membranes

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https://doi.org/10.1016/j.jcis.2025.01.224

We describe herein a cell membrane mimicking system designed for bioanalytical applications. Our tethered bilayer lipid membrane (tBLM) is based on mixed self-assembled monolayers (SAMs) on gold terminated by linear hydrophobic tethers. We studied the interfacial tBLM structure by employing neutron reflectometry (NR). Further on, as a proof of concept we have successfully reconstituted the deuterated outer membrane protein F (OmpF) from *E. coli* into our tBLM system and confirmed the protein insertion by NR. Thus, the presented cell membrane mimicking platform is promising for quantitative studies of lipid and protein structures and interactions taking place at the cell membrane.

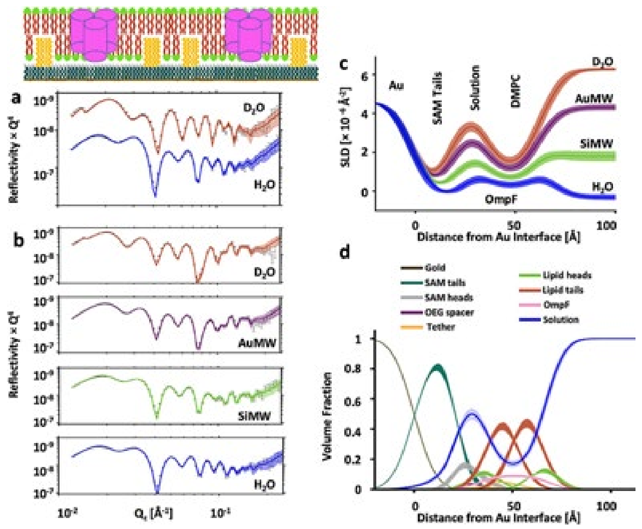
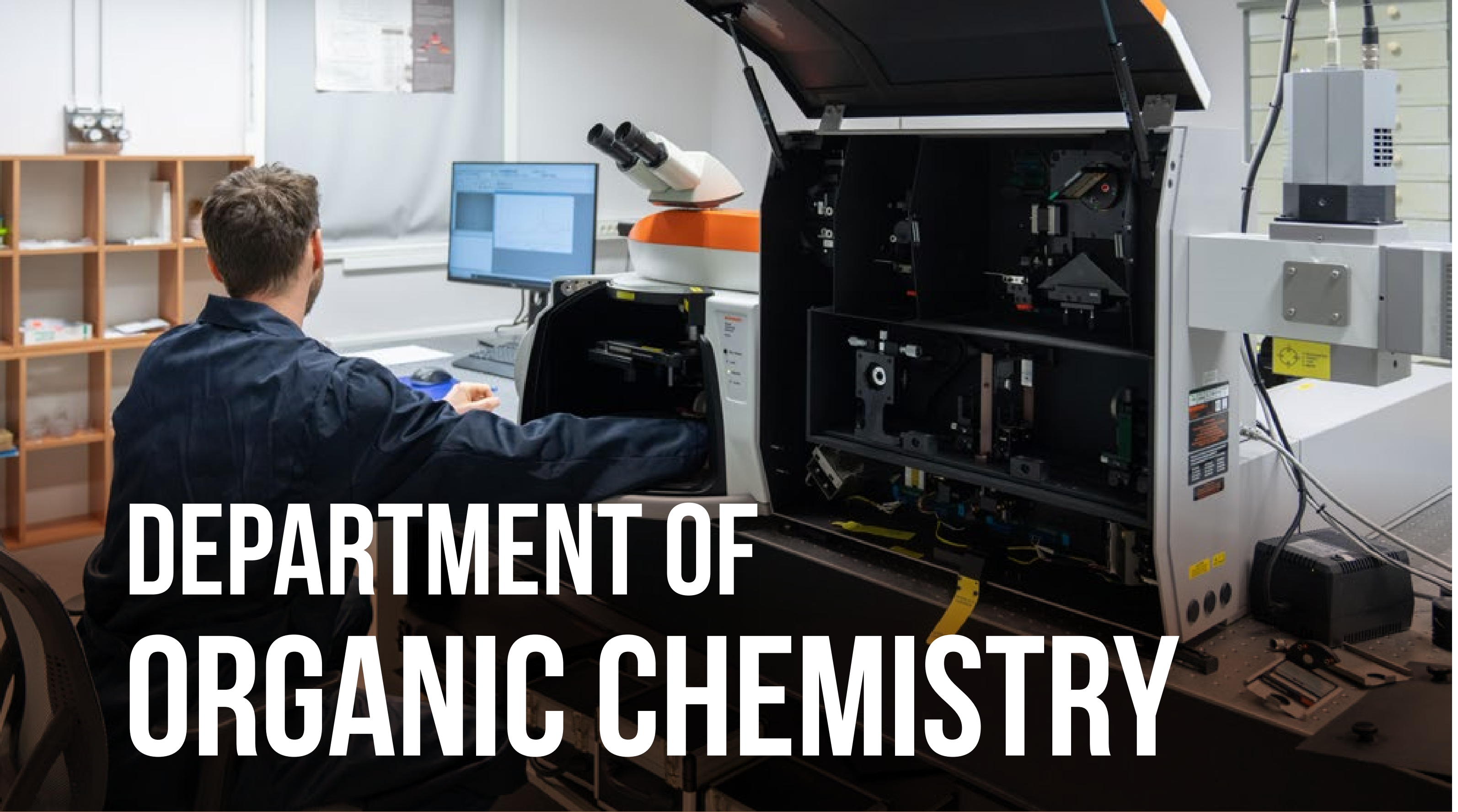


Fig. 3. Neutron reflectometry analysis of the protein-containing tethered lipid membrane.



DEPARTMENT OF ORGANIC CHEMISTRY

"Synthesis and analysis, surface modification and investigation, spectroscopy and electrochemistry - all in one"

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Surfaces and interfaces play a central role in electrochemical catalysis, energy conversion, electron transfer, and biochemical processes, requiring molecular-level insights into surface-adsorbed species. **The Spectroelectrochemistry Laboratory** is dedicated to the development and application of advanced spectroscopic and spectroelectrochemical techniques, enabling precise investigations of molecular adsorption, surface interactions, and electron transfer processes at interfaces. We employ multiwavelength Raman spectroscopy, surface-enhanced Raman scattering (SERS), resonance Raman spectroscopy (RRS), shell-isolated nanoparticle-enhanced Raman spectroscopy (SHINERS), and magneto-plasmonic nanostructure-enhanced Raman spectroscopy to investigate molecular-level changes induced by electrochemical potential in self-assembled molecular structures, 2D materials, and biological cells, including the ex vivo detection of kidney cancer biomarkers. Unique surface-sensitive techniques such as vibrational sum-frequency generation (VSFG) and surface-enhanced infrared absorption (SEIRA) spectroscopies are powerful tools for probing complex molecular systems and dynamics at interfaces with high sensitivity. These methods have been instrumental in studying the structural organization of lipid membranes, the interactions and dynamics of lipid-protein complexes, and the mechanisms by which membrane-damaging proteins impact membrane integrity and function. **The Laboratory of Organic Synthesis** focuses on advancing and applying fundamental organic chemistry to optimize the design and synthesis of molecules essential for research across diverse fields, including biology, biochemistry, medicine, pharmaceuticals, materials science, physics, optoelectronics, and semiconductors. The group specializes in the tailored synthesis of targeted compounds, prioritizing efficiency, cost-effectiveness, and high-quality output to meet the needs of both industrial and academic partners. This work supports applications ranging from biomedical research and drug development to advanced materials and electronic devices. **The Laboratory of Organic Analysis** develops, optimizes, and validates quantification methods using gas and liquid chromatography-mass spectrometry, aiming to enhance measurement system efficacy across various applications. Research includes essential oils from Lithuanian plants, VOCs and bioactive compounds in collaboration with other scientific institutes and private partners. Additionally, the laboratory emphasizes accuracy of chemical measurements and builds regional capacity for analytical chemistry, fostering innovations in academic and industrial applications.

Optimization of shell-isolated nanoparticle-enhanced Raman spectroscopy experiments with silver core-silica shell nanoparticles

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https://doi.org/10.1016/j.vibspec.2024.103666

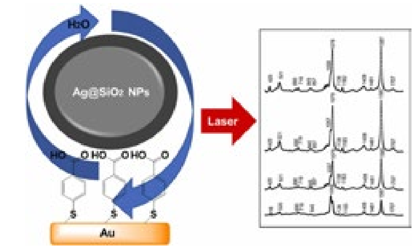

Fig. 1. Optimized silver core-silica shell nanoparticles for enhanced Raman spectroscopy

Silver core-silica shell nanoparticles (60–70 nm) have been optimized for Shell-Isolated Nanoparticle-Enhanced Raman Spectroscopy (SHINERS) experiments, enabling highly sensitive molecular analysis (Fig. 1). This research highlights an efficient synthesis method that avoids stabilizers, ensuring particle purity and stability. Optimized washing and dilution protocols improve Raman signal intensity, particularly for 4-mercaptobenzoic acid, a model analyte. These advancements make SHINERS more accessible for surface-sensitive molecular studies, from material science to biomedical applications. The findings pave the way for applying this methodology to other nanoparticle systems, enhancing the versatility and precision of spectroscopic analysis in research and industry.

Evaluation of physico-chemical characteristics of cement superplasticizer based on polymelamine sulphonate

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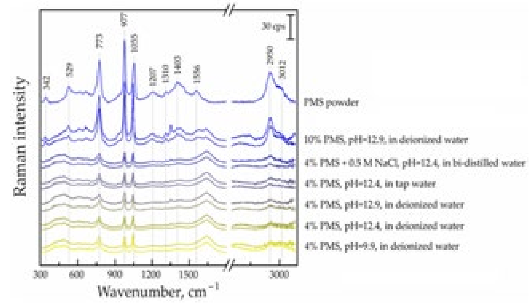

Fig. 2. Raman spectra of different polymelamine sulphonate (PMS) hydrolytic solutions (sampling time: 1 day and 3 years).

Polymelamine sulphonate (PMS)-based superplasticizers have been evaluated for their physicochemical stability in cementitious systems used in radioactive waste repositories. This research highlights the thermal stability of PMS up to 270 °C and its chemical resilience in highly alkaline environments (pH 9.9–12.9) over three years, verified using Raman and UV/Vis spectroscopy (Fig. 2). PMS enhances concrete properties by improving homogeneity, reducing water content, and increasing resistance to aggressive conditions. These findings support the long-term application of PMS in engineered barriers for radioactive waste management, ensuring durability and minimizing environmental risks. This study advances our understanding of polymer additives in challenging environments.

The research was funded by the European Joint Programme on Radioactive Waste Management, EURAD-CORI project (European Union's Horizon 2020 Research and Innovation Programme) under grant agreement No 847593.

Validation and application of an LC–MS/MS method for the determination of antioxidants originating from commercial polyethylene packages and their migration into food simulants

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A validated LC-MS/MS method was developed to analyze antioxidants, Irganox 1010 and Irgafos 168-ox, in commercial polyethylene food packaging and their migration into food simulants. The study revealed varying antioxidant levels and confirmed their migration into lipophilic and hydrophilic food simulants, with isooctane being the most aggressive (Fig. 3). Migration levels remained below regulatory limits (60 mg/kg), ensuring consumer safety. This work highlights the importance of precise analytical methods in assessing additive migration, aiding in regulatory compliance and improving food packaging safety. The findings contribute to understanding the interaction between polymer additives and food, addressing critical food safety concerns.

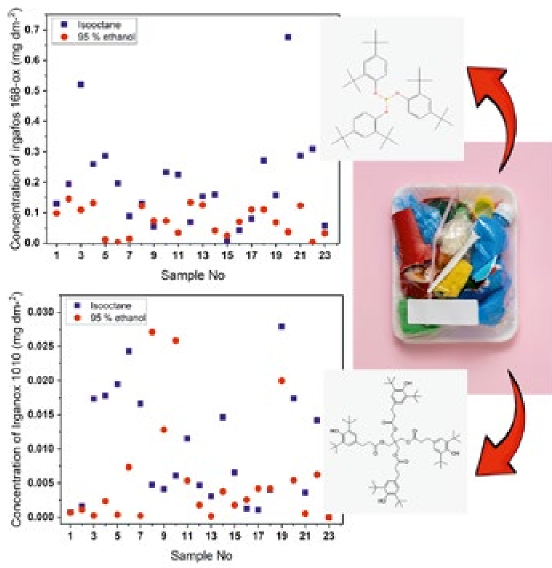
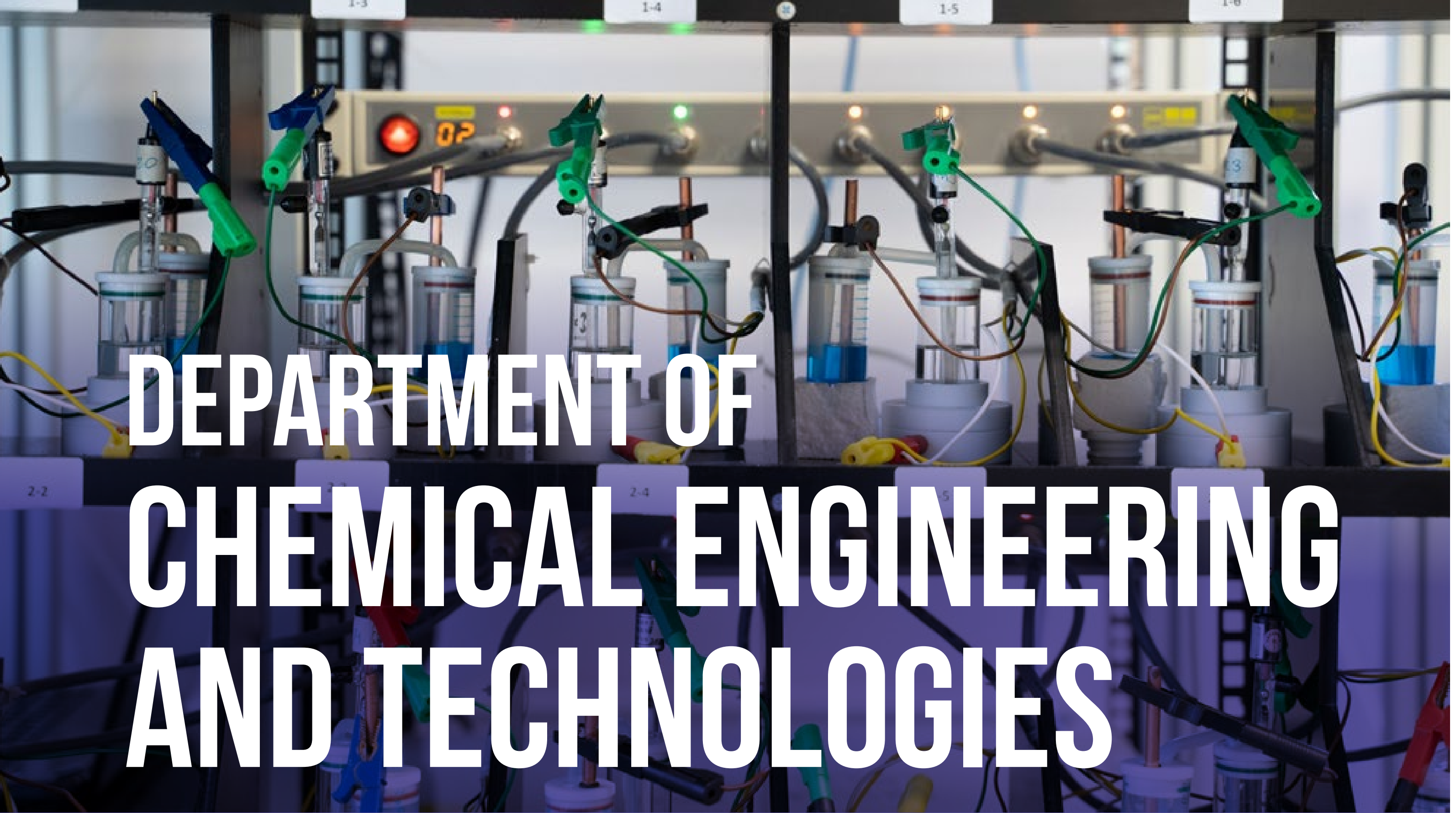


Fig. 3. Migration of Irgafos 168-ox and Irganox 1010 antioxidants originating from commercial polyethylene food packages.



DEPARTMENT OF CHEMICAL ENGINEERING AND TECHNOLOGIES

„Electrochemical technologies are pivotal in driving the transition to renewable energy and sustainable materials systems"

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The search for and development of novel energy conversion solutions are recognised as key tasks in modern science. Electrochemical energy conversion and storage technologies are attractive to many current renewable energy-related challenges. The primary activities of our department and its four laboratories (Electrochemical Energy Conversion, Tribology, Single-crystal Growth and Hazardous Waste Decontamination) focus on designing and developing functional materials, active surfaces, and interfaces for electrochemical energy conversion and circular economy. Extensive understanding and experience in electrochemistry and material science drive the development of innovative, sustainable technologies and new applications. The specific technologies developed in the department target the creation of safe, sustainable, and low-cost aqueous Na and Zn-ion batteries for stationary energy storage, light-driven electrochemical synthesis of hydrogen and strong oxidants suitable for water treatment and disinfection, and the valorisation of CO_2 through electrochemical reduction to valuable chemicals. Environmental friendliness, sustainability, and circularity are imperative for all newly developed technologies and potential applications.

The department is also active in the industrial scaling and application of anodic aluminium coatings and metallisation. Various characterisation techniques are widely applied and developed, emphasising the structural, morphological, and electrochemical properties of materials.

Lubrication of anodised aluminium

European Patent Application "Method for reactive impregnation of anodic alumina coating", No. EP23168208.9.
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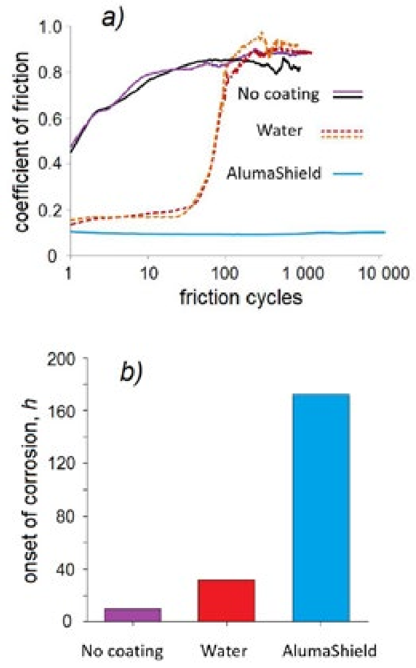
Low-wear anodised aluminium was invented by impregnating anodised surfaces with specific fillers for industrial applications such as pistons, bearings, rails, and other rubbing parts in mechanical systems. Hard (Type III) anodising of aluminium alloys is developed to produce nanoporous anodic coatings with thicknesses up to 100 µm or higher. Industrial aluminium alloys of 6000 and 7000 series are most preferable for anodising. Anodised aluminium surfaces are impregnated with our patented ***AlumaShield*** coating, which can penetrate into the nanopores of an anodic coating. Unlike barrier coatings, impregnated fillers within the nanopores can migrate into the friction zone, thus reducing the wear of anodised aluminium surfaces. ***AlumaShield*** impregnated surfaces also demonstrate high thermal stability up to 160°C. Combining the aluminium alloy and ***AlumaShield*** filler can improve the tribological performance of anodic coatings 20 times or more compared to commercial lubricants.



Nanostructured porous WO_3 for photoelectrochemical splitting of seawater

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Due to its salinity, seawater can serve as an electrolyte in photoelectrochemical (PEC) systems, potentially enabling a solar-driven production of hydrogen and oxidising species. In this study, several micrometres thick and highly porous nanostructured WO_3 films were formed, and their performance in photoanodic oxidation of chloride and sulphate ions, the most abundant anionic species in seawater, was investigated (Fig. 1). The study demonstrates that efficient PEC performance is achieved through optimal light absorption by sufficiently thick WO_3 layers (3-5 µm). This highly porous structure facilitates electrolyte permeation and ionic transport and provides a large electrochemically active interfacial area, as well as a nanosheet morphology where the sheet thickness is shorter than the hole diffusion length in WO_3. The Faradaic efficiency of reactive chlorine species (ClO^-+ClO_2^-) generation in neutral chloride-based electrolytes was close to 100%, whereas the presence of sulphate ions did not affect the formation of reactive chlorine species. The findings of the study suggest that thick nanoporous WO_3 layers are potential candidates to be used in the photo-electrolysis of saline water for efficient light-driven production of chlorine-based oxidants suitable for water treatment and disinfection.

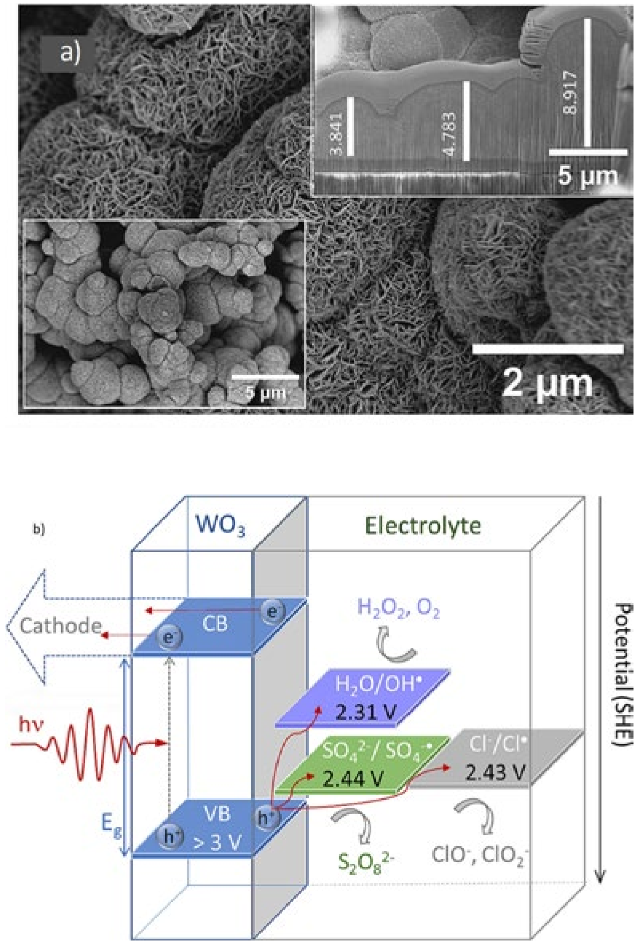

Fig. 1. (a) SEM images of nanostructured WO_3 films; (b) a schematic representation of possible hole-induced photoanodic processes occurring at WO_3 photoanode in aqueous chloride and sulphate solutions.

Reducing electrolyte additives for preparing capacity-balanced aqueous Na-ion battery cells

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The invention relates to an electrochemical energy storage cell containing an aqueous electrolyte solution. Positive and negative electrodes of an electrochemical cell are composites comprising ion-insertion materials capable of reversible insertion and extraction of ions. The electrochemical storage cell contains an aqueous electrolyte solution and comprises a reductive additive such as hydrazine added at low concentration. Adding the reducing agent into the aqueous electrolyte solution suppresses parasitic reactions, allowing the manufacturing of electrode capacity-balanced cells with a positive versus negative electrode charge capacity ratio equal to unity. The balanced electrode charge capacity ratio and the absence of self-consuming electrode charge overcapacity improve cycle lifetime and reduce the self-discharge of such electrochemical cells (Fig. 2).

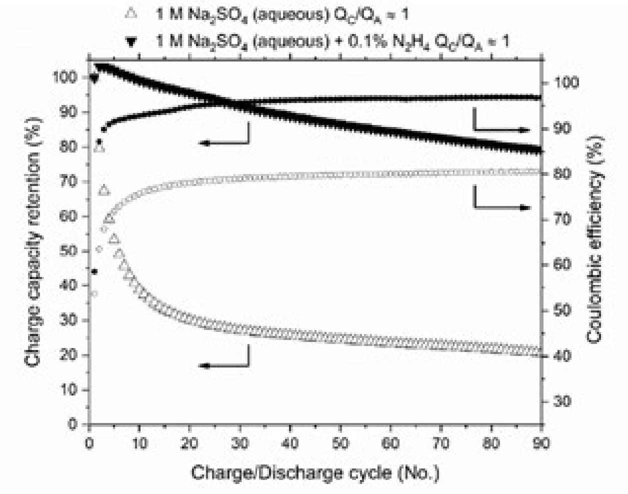

Fig. 2. The relative capacity retention and Coulombic efficiency of two symmetric $Na_2VTi(PO_4)_3|Na_2VTi(PO_4)_3$ coin cells with electrode charge capacity (N/P) ratio of ~ 1 using 1 M Na_2SO_4 (aq.) electrolyte with and without hydrazine.

Wear resistance and antibacterial properties of 3D-printed Ti6Al4V alloy after gas nitriding

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https://doi.org/10.1016/j.triboint.2024.109839

This research focused on tribological and antibacterial studies of 3D-printed Ti6Al4V alloys, based on the selective laser melting method vs conventional technology, after gas nitriding for biomedical applications. Gas nitriding reduced friction and wear in the following order: 3D-printed AM Ti6Al4V > wrought CM Ti6Al4V > CP-Ti. The best tribological performance was demonstrated on nitrided Ti6Al4V alloy using 3D printing. The antibacterial activity of the samples was estimated for the Gram-positive *Staphylococcus aureus* and the Gram-negative bacteria *Escherichia coli*. The AM Ti6Al4V showed a positive antibacterial effect of nitriding against S. aureus bacteria by up to 30 % (Fig. 3). Gas nitriding of 3D-printed Ti6Al4V alloys suggests an effective strategy to improve the antibacterial activity and mechanical resistance of biomedical implants.

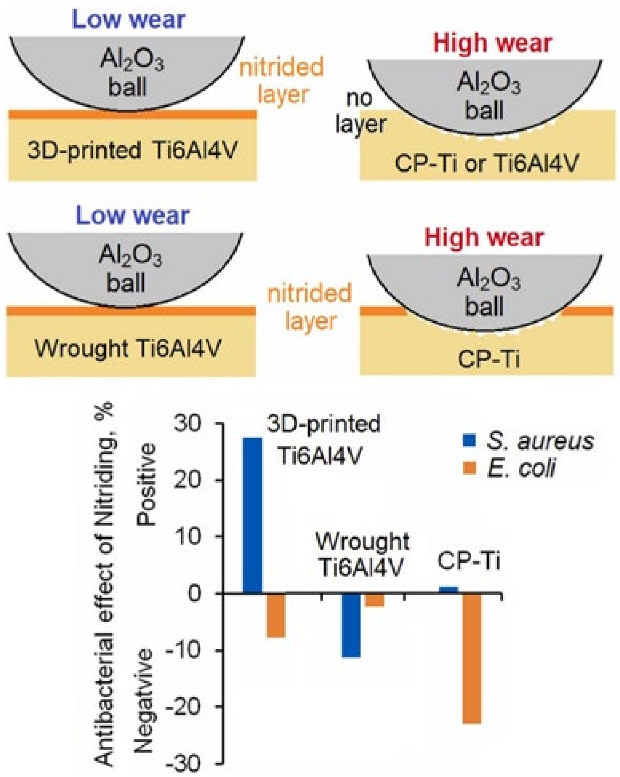

Fig.3. Wear resistance of 3D-printed Ti alloys vs conventional manufacturing before and after gas nitriding (top) and antibacterial effect of nitriding against *S. aureus* and *E. coli* bacteria (bottom).

Firefighting wastewater from a tire recycling plant: Chemical characterisation and simultaneous removal of multiple pollutants

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Large volumes of wastewater were produced after extinguishing the uncontrolled burning of used tires in one of the biggest tire recycling companies in the Baltics in 2019. Chemical analysis of the generated firefighting wastewater (FW) was performed, and significant FW contamination was identified. More than one hundred organic pollutants belonging to different classes were detected by HPLC, GC/FID, and GC/MS, including PAHs (14.2 μg/L) and VOCs (15.3 μg/L) (Fig. 4). ICP-OES revealed high levels of heavy metals, especially zinc and manganese, with 580 and 1213 μg/L Zn and Mn, respectively. Six commercial activated carbons (ACs) and polymer adsorbent MN 200 were tested for FW treatment in batch mode. According to the pollutants removal efficiency (RE), the Norit Row 0.8 Supra, the most appropriate adsorbent for the simultaneous removal of total heavy metal and organic pollutants from FW, has been selected (Fig. 5). It was found that AC reduced the concentration of organic pollutants in FW to 85% within 1 h in batch. Pb was the most adsorbed heavy metal, regardless of the mode of adsorbent operation. The time-dependent behaviour of AC in the pollutant's removal in the fixed-bed column was described using a mass transfer model. Retention of organic matter to the 50% breakthrough point took nearly three times longer than that of heavy metal ions. After pre-treatment with activated carbon, the FW can be directed to a municipal sewage treatment plant.

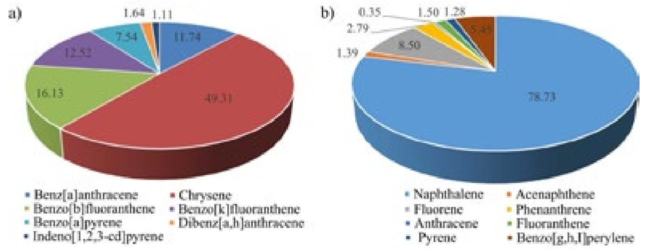


Fig. 4. Percentage distribution of polycyclic aromatic hydrocarbons in the Alytus FW: (a) carcinogenic PAHs; (b) potential carcinogenic PAHs.

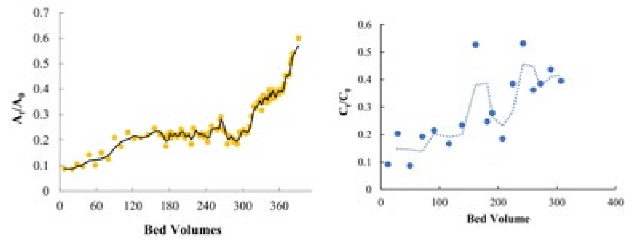
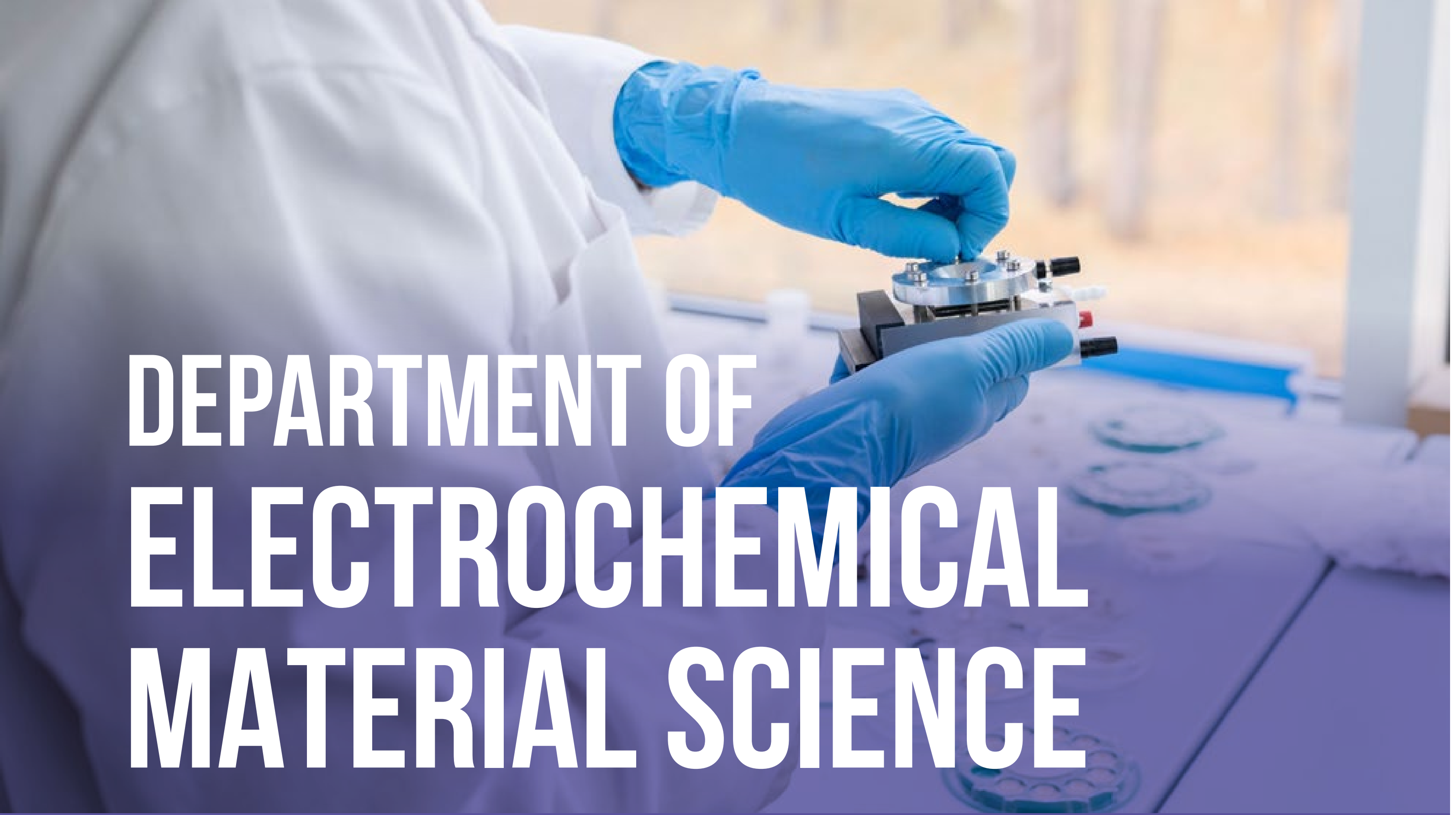


Fig. 5. (a) Removal of organic pollutants and (b) simultaneous the total heavy metal removal (Σ=Pb+Zn+Co+Cu+Mn) from FW in a fixed-bed column filled with activated carbon Norit Row 0.8 Supra. At/A0 is the normalised concentration of pollutants according to the UV-absorbance data at the wavelength 254 nm; C_t/C_0 is the normalised total concentration of heavy metals.



DEPARTMENT OF ELECTROCHEMICAL MATERIAL SCIENCE

"Material science is one of the most promising fields that will not lose its relevance, as no matter what topic we discuss, we always encounter material-related challenges"

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The Department's Nanostructure Laboratory and Materials Science and Corrosion Laboratory focus on applying electrochemical methods to develop and characterise new materials and technologies for energy conversion, photocatalysis, nanomedicine, and material degradation control.

Key research activities in the Materials Science and Corrosion Laboratory include the electrochemistry of silicon and other semiconductors, particularly the electrochemical synthesis of nano- and microstructures on silicon. These structures are applied in sustainable energy technologies, such as photovoltaics, hydrogen photogeneration, and next-generation batteries. Another significant focus is the development of nano-thin semiconductor layers, utilising techniques such as electrochemical deposition, PVD, and ALD to enhance photo- and electrocatalytic reactions and control degradation through transparent and electrically conductive films.

The Nanostructure Laboratory specialises in synthesising and characterising novel nanomaterials for applications in optoelectronics, materials engineering, and energy. This includes work on superparamagnetic and luminescent nanoparticles with potential applications in nanomedicine. Additionally, research on nanostructured titania, gold, and iron oxide layers involves optimising formation processes, modifying composition, and functionalising surfaces for specialised uses.

The Materials Science and Corrosion Laboratory also conducts expert and accredited assessments of metal corrosion in electrolytes, as well as in natural and artificial atmospheres, alongside the development of advanced corrosion protection technologies.

New process for the formation of mixed-valence platinum sulphide thin films from bulk CdS layer: characterization of physical and electrochemical properties

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https://doi.org/10.1021/acsaem.3c03185

A thin film (60-90 nm) of mixed-valence platinum sulphide (PtSM) has been successfully deposited on a fluorine-doped tin oxide substrate. An innovative method was developed to synthesise this film in which Cd atoms were replaced by Pt atoms within the bulk of a CdS layer prepared by chemical bath deposition. The PtSM films were analysed using various characterisation techniques, such as Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), and X-ray diffraction (XRD). The analysis revealed that PtSM films mainly compromise PtS, PtS_2, and a small amount of CdS. The surface composition of PtSM films was determined by XPS analysis, which indicated that the composition consists of 73.8% PtS and 26.2% PtS_2. The detailed sequence and mechanism of PtSM film formation were investigated using electrochemical, photoelectrochemical, and Mott–Schottky analysis. The hydrogen evolution reaction (HER) properties of the films were also investigated. In a 1.3 M lactic acid and 0.25 M Na_2SO_4 solution at pH 2, the best PtSM film and Pt metal electrode showed HER electrocatalytic performance with overpotentials of −0.317 and −0.267 V, respectively, at a current density of −10 mA cm^{-2}. A long-term stability test demonstrated that the film is stable and not subject to degradation. The practical application of the PtSM coating was demonstrated by photoelectrochemically induced HER on PtSM-coated p-Si wafers.

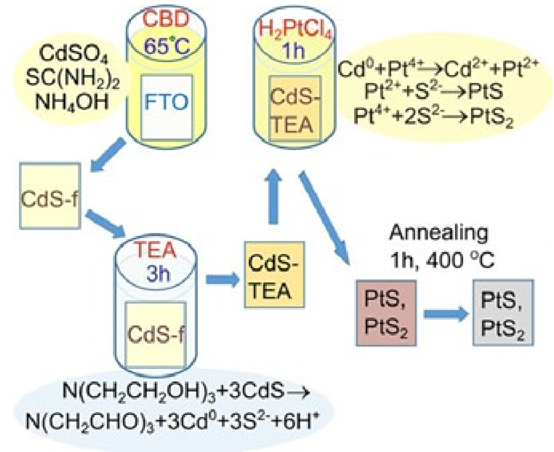

Fig. 1. Process of deposition of mixed valence platinum sulphide film.

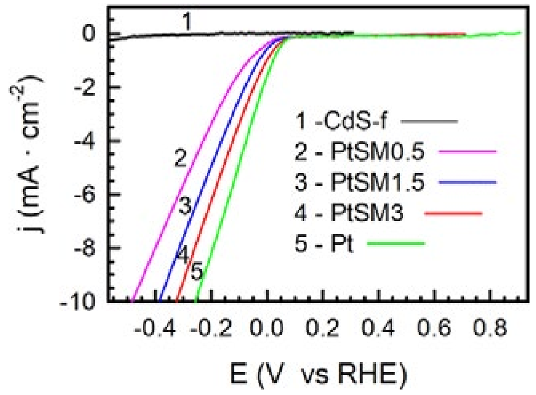

Fig. 2. Linear sweep voltammograms of cadmium sulphide (CdS-f), mixed valence platinum sulphide prepared at various conditions (PtSM0.5, PtSM1.5, PtSM3) and platinum (Pt) at a scan rate of v = 20 mV s^{-1} in the dark for the hydrogen evolution reaction.

The enhancement of hydrogen evolution reaction on nanoplatelet-shaped MoS_2 via anodic pretreatment

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This work presents the effect of anodic pretreatment of 2D-MoS_2 nanoplatelet-shaped films hydrothermally synthesised on the anodised Ti substrate for electrocatalytic H_2 evolution from water. The growing hydrogen evolution reaction efficiency upon anodic pretreatment was ascribed to increased sulphur content in the MoS_2 nanoplatelet edges in the form of more active bridging S_2^{2-} and apical S^{2-} groups.

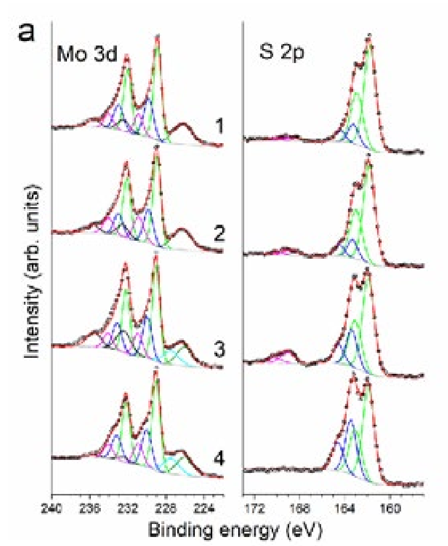

Fig. 3. Deconvoluted XPS plots for Mo 3d and S 2p states of MoS_2 samples treated for 900 s at +0.10 V (1), +0.30 V (2), +0.60 V (3), +0.80 V (4)).

A 2D-to-3D morphology transitions of gold in organic acid electrolytes: characterisation and application in bioanode design

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https://doi.org/10.1016/j.apsusc.2023.158654

This work introduces a novel, simple and cheap approach for 2D gold surface morphology transitions into porous 3D nanostructures. This gold transition can be achieved using an electrochemical anodisation technique of any bare gold, including disposable screen-printed electrodes (1 in Fig. 4). Compared to traditional chemical dealloying of gold alloys, this method is beneficial because it can be done in non-aggressive electrolyte solutions such as oxalic and glycolic acids. This feature could benefit practical uses because it does not destroy the other parts of the SPE electrode (i.e. Ag-pseudo reference electrode) and results in smaller nanostructure formation. After anodisation in oxalic and glycolic acids, the traditional colour of gold changes into black or grey-black, evidencing the nanoscale-sized surface morphology (2). To date, glycolic acid has never been utilised to anodise gold.

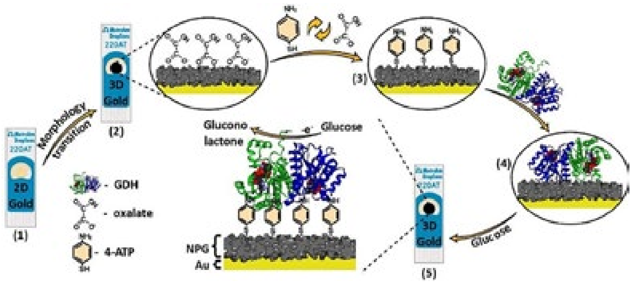

Fig. 4. Process of gold surface morphology transition and bioanode construction.

Additionally, the designed nanoporous gold (NPG) surfaces were shown to be suitable for the development of bioanode. To enhance direct electron transfer (DET)-type bioelectrocatalysis, we immobilised 4-amino thiophenol self-assembly monolayers on the NPG surfaces (3). Then, electrodes were enriched with glucose dehydrogenase enzyme (4). The constructed bioanode (5) exhibited high current and power densities, which were much higher if the NPG structures were formed in glycolic acid solutions.

Possibility of phase transformation of Al_2O_3 by a laser: a review

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https://doi.org/10.3390/cryst14050415

High-quality aluminium (Al) components often require an optimal ratio of lightness and favourable mechanical properties. To improve the physical-mechanical properties of Al, an aluminium oxide (Al_2O_3) film is usually formed on the surface of Al, which itself is characterised by high strength, hardness, corrosion resistance, and other technical properties. Unfortunately, depending on the conditions, the oxide film may be formed from different crystal phases on the Al surface, which are not always of desirable quality, i.e., the α-Al_2O_3 phase. The present review demonstrates that the properties of the Al_2O_3 film may be improved by Al processing with a laser beam according to the scheme: Al (Al alloy) → electrochemical anodising → treatment with laser irradiation → α-Al_2O_3. Both, the Al substrate and the anodising electrolyte, affect the phase transformation of anodic Al_2O_3. Laser irradiation of the Al_2O_3 surface leads to high heating and cooling rates, which may promote the formation of a highly crystalline α-Al_2O_3 phase on anodic Al_2O_3.

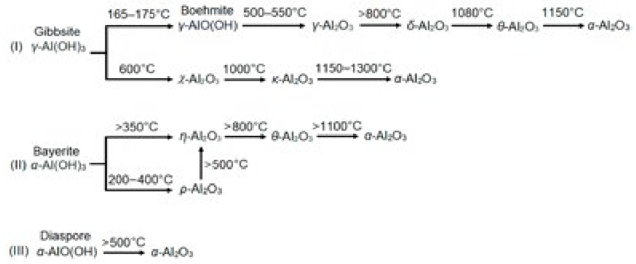
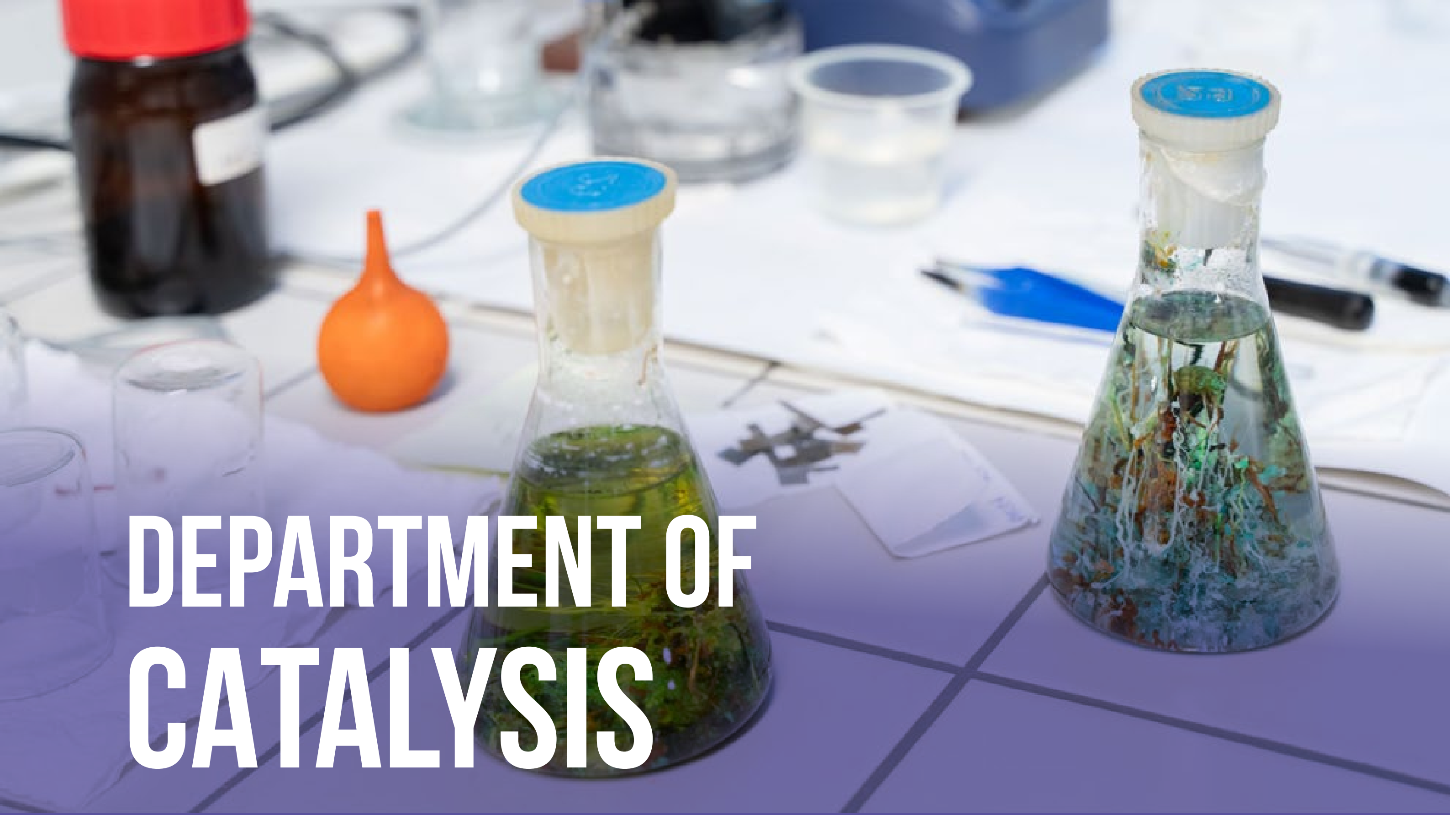


Fig. 5. Structure and phase transformations of aluminium oxides and aluminium hydroxides.



DEPARTMENT OF CATALYSIS

„High-performance multifunctional catalytic materials for sustainable catalysis"

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The R&D activities at the Department of Catalysis are focused on developing advanced catalytic materials and processes. The research includes designing and developing high-performance multifunctional catalytic materials using various techniques, including electroless and/or electrochemical metal plating, dynamic hydrogen bubble template, microwave, and hydrothermal synthesis techniques. Coatings of noble and base transition metals and their alloys with different structures, compositions and very high electrochemically active surface areas have been developed and deposited on a variety of conductive and non-conductive flexible substrates (metals and their rigid foams, polymers: polyethylene (PE), polypropylene (PP), polyvinyl chloride, polyimide, polyethermides), silicon carbide, quartz particles, using the electroless metal plating method. The R&D activities in this area are focused on the development of novel electroless metal plating processes as well as fundamental studies of the reactions occurring in autocatalytic metal ions reduction systems using electrochemical quartz crystal microgravimetry and their application in microelectronics, renewable and low-carbon energy conversion and storage technologies, such as chemical and electrochemical hydrogen production, low-temperature fuel cells, metal-air batteries and supercapacitors, etc. Electroless metal plating is a method for depositing 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 metallisation. Selecting suitable reducing agents and reaction conditions (temperature, the concentration of the reacting substances, etc.) plays a vital role in creating stable solutions and obtaining coatings with required properties, such as purity and surface roughness. Researchers in the Department of Catalysis are experienced in studying the electrocatalytic activity of engineered materials for a variety of catalytic reactions using electrochemical techniques such as cyclic voltammetry, chronoamperometry, chronopotentiometry, rotating disk electrode (RDE) and ring-disk electrode (RRDE), and electrochemical impedance spectroscopy (EIS) methods. Another important topic in the Department of Catalysis is the development of commercially viable and efficient biochar materials from wastes of the wood industry, biorefineries, and the pulp and paper industry. The synthesised novel high-performance, high-conductivity, electrocatalytically active, durable, low-cost, high-surface-area carbon materials with controlled pore size distribution have been successfully applied as electrode materials in supercapacitors, metal-air batteries and fuel cells.

MnO_2 nanoparticles supported on graphitic carbon nitride as an electrocatalyst for oxygen reduction and evolution

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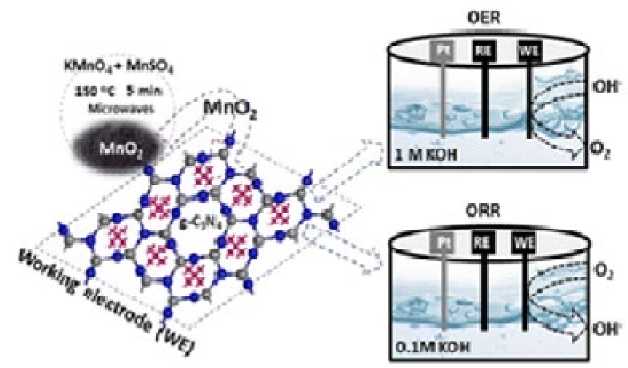
This study presents a straightforward methodology for the preparation of non-precious metal catalysts comprising MnO_2 and carbonaceous materials, namely graphite powder (C), graphitic carbon nitride (gCN), and graphitic carbon nitride/graphite powder (gCN/C) substrates. The investigated catalysts exhibited enhanced electrocatalytic activity with regard to the ORR and OER processes when compared with the bare substrates. The MnO_2–gCN/C catalyst was found to be the most efficient catalyst for both investigated reactions when compared with MnO_2/C and MnO_2–gCN. The MnO_2–gCN/C catalyst demonstrated the most positive ORR onset potential of 0.9 V and the most negative OER onset potential of 1.53 V. Furthermore, it demonstrated remarkable stability, retaining approximately 85% of its initial signal after a continuous test of 24 hours in both long-term ORR and OER processes.



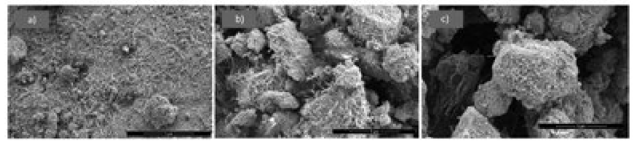


Fig. 1. SEM images of MnO_2/C (a), MnO_2-gCN (b), and MnO_2-gCN/C (c).

Plasma electrolytic oxidation synthesis of heterostructured TiO_2/Cu_xO films for photoelectrochemical water splitting applications

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This study presents the synthesis of TiO_2 films by an anodization-like procedure called plasma electrolytic oxidation (PEO). Different morphologies and structures were obtained by varying synthesis conditions. Moreover, successful heterostructuring was achieved by adding a copper precursor to the solution. Structural, optical, and photoelectrochemical properties of the TiO_2/Cu_xO films were characterised. Overall, the heterostructures were found to generate larger photocurrents, most likely due to a combination of their improved crystallinity and lower band gaps. Mott-Schottky analysis confirmed that the Vfb values of the TiO_2/Cu_xO films became more positive with increasing copper content, and the data was cross-referenced to Gartner-Butler plots and observations from PEC measurements. The photoanode performance of all films was improved by adding methanol, which acted as a hole scavenger, and IMPS spectra revealed that this improvement could be related, at least in part, to the elimination of surface electron-hole recombination.

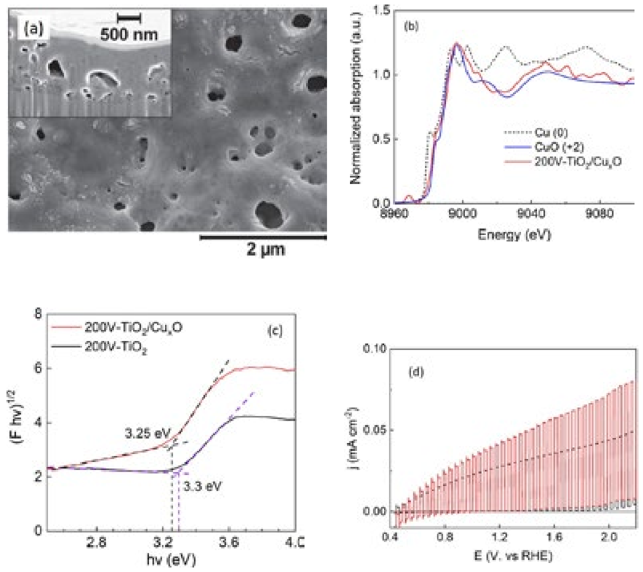

Fig. 2. (a) SEM image of TiO_2/Cu_xO film; (b) XANES spectra of films; (c) Tauc plots for TiO_2 and heterostructured film; (d) Chopped-light linear sweep voltammograms of TiO_2 and heterostructured film in 1 M KOH.

3D nickel-manganese bimetallic electrocatalysts for an enhanced hydrogen evolution reaction performance in simulated seawater/ alkaline natural seawater

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https://doi.org/10.1016/j.ijhydene.2024.07.131

This work presents a novel self-supported bimetallic NiMn/Ti electrocatalyst with a porous architecture and uniform metal dispersion, which enables highly efficient and stable hydrogen evolution reaction (HER) via seawater splitting. The catalyst was synthesised by a simple and eco-friendly one-step electrochemical deposition method using a dynamic hydrogen bubble template technique. The best NiMn/Ti electrocatalyst exhibited superior HER activity and stability, requiring ultra-low overpotentials of 64.2 and 79.3 mV to achieve the benchmark current density of 10 mA cm^{-2} in simulated seawater and alkaline natural seawater, respectively, which are highly comparable to most of the non-noble metal-based electrocatalysts reported in the recent past. The results highlight the potential of this cost-effective electrocatalyst for advancing sustainable hydrogen production from natural seawater.

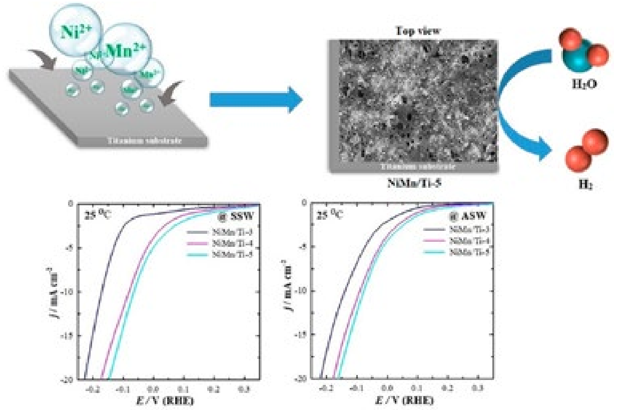

Fig. 3. HER polarisation curves of 3D NiMn/Ti catalysts in simulated seawater and alkaline natural seawater at 10 mV s^{-1} potential scan rate at 25°C temperature.

Pd and Ni nanoparticles on N-doped graphene from upcycled water bottle waste as an effective fuel cell electrocatalyst

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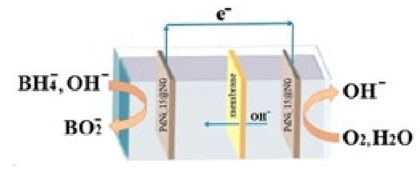
Environmental pollution due to the excessive consumption of fossil fuels for energy production is a critical global issue. Fuel cells convert chemical energy directly into electricity in a clean and silent electrochemical process but face hydrogen storage, handling, and transportation challenges. The direct borohydride fuel cell, which uses sodium borohydride as a liquid fuel, is a promising alternative to overcome such issues but requires the development of cost-effective nanostructured electrocatalysts. In this study, nitrogen-doped graphene-anchored Ni nanoparticles (Ni@NG) were synthesised by thermal degradation of polyethylene terephthalate bottle waste with urea and metallic Ni and evaluated as a sustainable carbon support. Electrocatalysts were prepared by incorporating low amounts (0.5 to 1.5 wt.%) of Pd into the Ni@NG support. The electrocatalytic activity of the materials for oxygen reduction and borohydride oxidation reactions in alkaline media, corresponding to the anodic and cathodic reactions in DBFCs, was evaluated by voltammetry. The electrocatalyst with the highest Pd content (PdNi_15@NG) exhibited the best performance for both reactions. Consequently, it was employed as the anode and cathode material in a laboratory-scale DBFC, achieving a specific power of 3.46 kW g_{Pd}^{-1}.



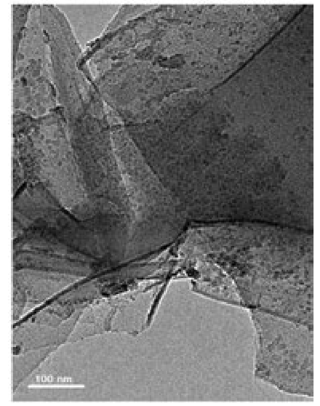


Fig. 4. Schematic diagram of the assembled direct borohydride fuel cell and TEM image of PdNi15@NG.

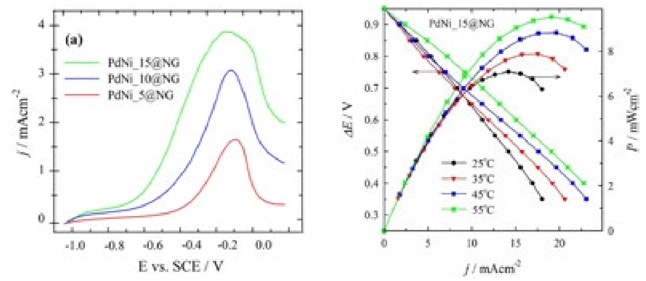
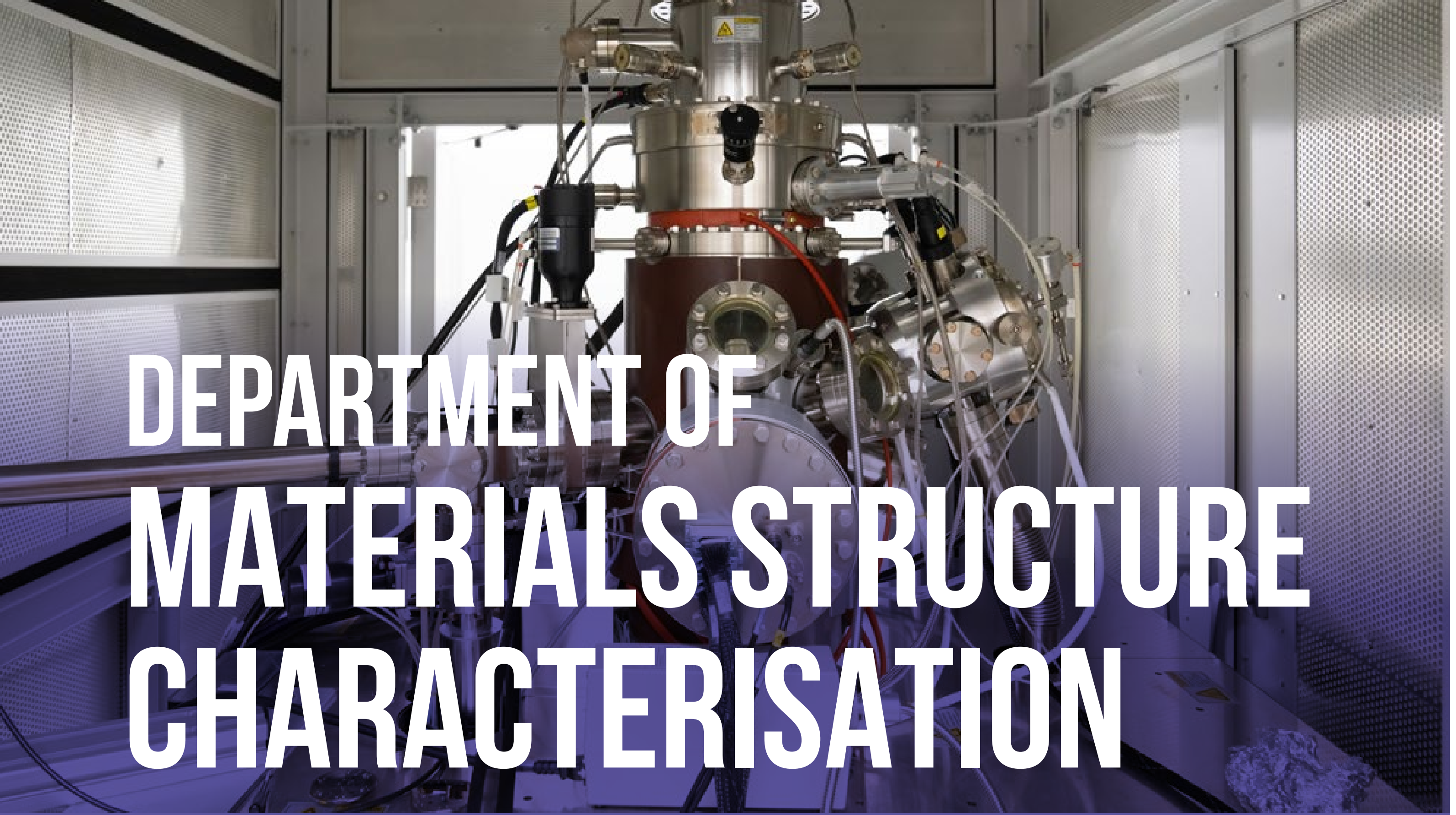


Fig. 5. (a) Comparison of forward scans of PdNi_5@NG, PdNi_10@NG, and PdNi_15@NG catalysts in 0.03 M $NaBH_4$ + 2 M NaOH at 50 mV s^{-1}; 25 °C. (b) Cell polarisation and corresponding power density curves for a DBFC using PdNi_15@NG as anode and cathode electrocatalysts in 1 M $NaBH_4$ + 2 M NaOH anolyte and O_2-saturated 1 M NaOH catholyte at temperatures ranging from 25 to 55 °C.



DEPARTMENT OF MATERIALS STRUCTURE CHARACTERISATION

„Although department is small, it plays a vital role in aiding to develop various technologies raging from catalysis, energy materials to optical coatings and quantum structures"

Dr. Rokas Kondrotas

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The department is divided into two laboratories: the research area of the first laboratory is focused on the in-depth characterisation of materials structure by various microscopic and spectroscopic methods. The goal is to provide a comprehensive analysis of materials' crystalline structure, morphology, chemical and phase compositions. Various samples varying from epitaxial thin films to material composites, crystalline powders or nanoparticles are studied and analysed. The research field of the second laboratory entails the synthesis and study of chalcogenide materials for optoelectronic application with a special focus on the development of sustainable thin film solar cells. The goal is to develop chalcogenide-based wide and narrow bandgap technologies for application in flexible, indoor, semi-transparent and multijunction photovoltaic devices.

Synthesis and characterisation of polycrystalline GeS thin films for optoelectronic applications

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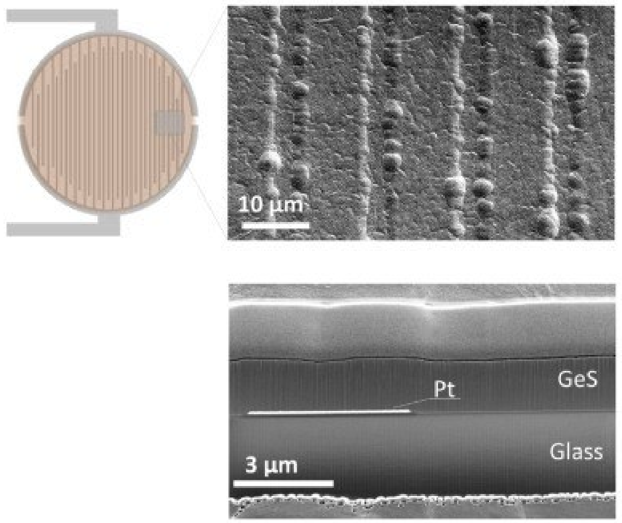
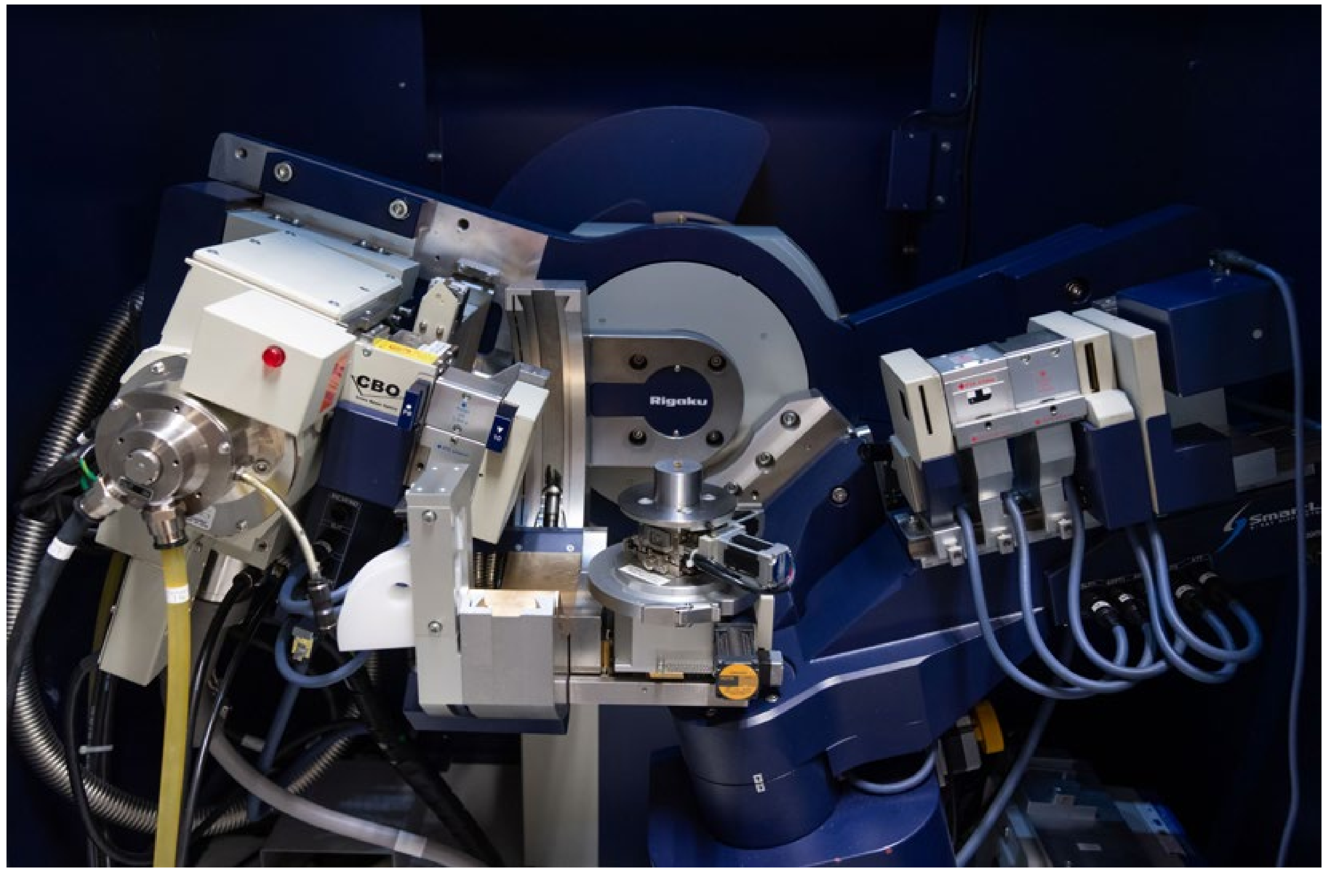
https://doi.org/10.1016/j.mssp.2024.109193

The search of novel materials with more environmentally benign composition and processing play an important role in development of sustainable optoelectronic technologies in the future. Layered semiconductors are promising for new optoelectronic applications due to their unique optical and electronic properties. This study focuses on the synthesis of thin germanium monosulphide (GeS) films and the characterization of their structural and optoelectrical properties. Authors develop a simple two-step deposition process for producing highly crystalline and with controlled thickness and texture GeS thin films. Photoelectric characterization using current-voltage characteristics, transient photocurrent and time-delayed collection field measurements revealed that polycrystalline GeS is a photosensitive material with long carrier lifetimes and therefore promising for optoelectrical applications.





DEPARTMENT OF NANOTECHNOLOGY

„Nano-scale structures on top of electrode have an enormous and diverse potential on sensitivity and selectivity of electrochemical, optical, acoustic, or biological sensors"

Prof. Hab. Dr Arūnas Ramanavičius

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The main research directions in the Department of Nanotechnology are related to developing sensors, biosensors, immuno-analytical systems, molecularly imprinted polymer-based sensors, and other related research directions. The most extensive experiments of the Department of Nanotechnology are dedicated to developing optical, acoustic, and electrochemical sensors for detecting SARS-CoV-2 proteins. Spectroscopic ellipsometry and quartz crystal microbalance methods are used to research optical and acoustic biological sensors.

To gain sensitivity to SARS-CoV-2 proteins, electrochemical sensors were modified with self-assembled monolayers or conducting polymers (including molecularly imprinted polymers). Such sensors are researched using differential pulse voltammetry, cyclic voltammetry, pulsed amperometric detection, and other electrochemical methods.

In the laboratory of bioelectrochemical technologies, we develop and research biofuel cells and biological sensors. We are also developing a scanning electrochemical microscope using artificial intelligence and image recognition to create user-friendly measurement equipment that can be easily adapted to different objects and environments.

Design of molecularly imprinted polymers using computational methods: a review of strategies and approaches

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https://doi.org/10.1002/wcms.1713

This paper focuses on the computationally assisted design of molecularly imprinted polymers (MIP), emphasising the selected strategies and chosen methods of approach. In summary, this paper provides an overview of the MIP fabrication procedure, focusing on key factors and challenges, where the fabrication of MIP includes a step-by-step process with extensive experimental procedures (Fig. 1). This brings challenges in optimising experimental conditions, such as the selection of monomer, cross-linker, and their relevant molar ratios to the template and solvent. Next, the principles of computational methods are elucidated to explore their potential applicability in solving the challenges. The computational approach can tackle the problems and optimise the MIP's design. Finally, the atomistic, quantum mechanical (QM), and combined methods in the recent research studies are overviewed with emphasis on strategies, analyses, and results. It is demonstrated that optimisation of pre-polymerization mixture by employing simulations significantly reduces the trial-and-error experiments. Besides, higher selectivity and sensitivity of MIP are observed. The polymerisation and resulting binding sites are considered by computational methods. Several models of binding sites are formed and analysed to assess the affinities representing the sensitivity and selectivity of modelled cavities. Combined QM/atomistic methods showed more flexibility and versatility for realistic modelling with higher accuracy. This methodological advancement aligns with the principles of green chemistry, offering cost-effective and time-efficient solutions in MIP design.

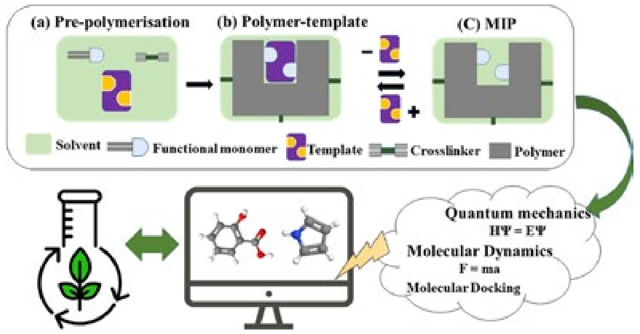

Fig. 1. Schematic representation of the MIP preparation steps.

Application of computational methods in the design of molecularly imprinted polymers (review)

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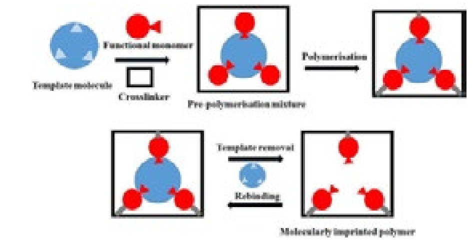
The potential of computational methods (molecular mechanics, molecular dynamics, Monte Carlo simulations, quantum mechanics, and statistical simulations) in designing molecularly imprinted polymers (MIPs) to avoid costly trial-and-error experiments and better understand the processes at each step is demonstrated. The preparation of MIPs step-by-step and the demonstration of numerous examples of how the computational methods were applied to solve emerging challenges are overviewed (Fig. 2). The selection of chemicals, including monomers, solvents, and cross-linkers, by different computational means is discussed. In silico modelling of the polymerisation step effectively simulates the fabrication of the MIPs. Combining these findings makes creating polymeric structures with imprinted binding sites feasible. Research studies that employed computational methods for evaluating MIP selectivity and recognition ability and the results are overviewed. The examined studies proved the significance and the functionality of computational methods for MIP design.

Fig. 2. Scheme of the preparation of molecularly imprinted polymers.



Microbial fuel cell based on *Ensifer meliloti*

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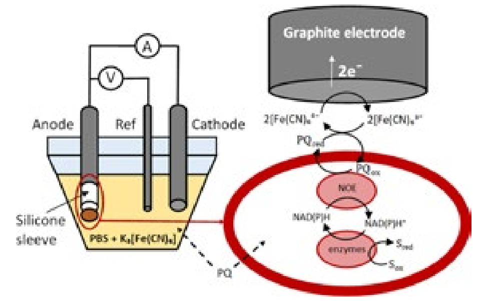
The world's growing energy crisis demands renewable energy sources. This issue can be solved using microbial fuel cells (MFCs). MFCs are biocatalytic systems that convert chemical energy into electrical energy, reducing pollution from hazardous chemical compounds. However, during the development of MFCs, one of the most significant challenges is finding and assessing microorganisms that generate sufficient redox potential through metabolic and catalytic processes. In this research, we have used *Ensifer meliloti (E. meliloti)* bacteria to design MFCs based on consecutive action of two redox mediators (9,10 - phenanthrenequinone (PQ) and potassium ferricyanide), which transferred charge between *E. meliloti* bacteria and graphite rod electrode. A viability study of *E. meliloti* culture showed that PQ significantly inhibits the growth of bacteria at 0.036 mM. Cyclic voltammograms were registered in the presence of 20 mM potassium ferricyanide and different concentrations (0.036 and 0.071 mM, 0.11 mM, 0.14 mM, 0.172 mM, 0.32 mM) of PQ. Four days of lasting assessment of the microbial fuel cells in two-electrode systems showed showed that the maximal open circuit potential and the power increased during the experiment from 174.9 to 234.6 mV and from 0.392 to 0.741 mW m^{-2}, respectively.

Fig. 3. Schematic diagram of a single-chamber microbial fuel cell based on *Ensifer meliloti* grown on graphite rod electrode structure.



Monitoring $Ti_3C_2T_x$ MXene degradation pathways using Raman spectroscopy

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Extending applications of $Ti_3C_2T_x$ MXene in nanocomposites and across fields of electronics, energy storage, energy conversion, and sensor technologies necessitates simple and efficient analytical methods. Raman spectroscopy is a critical tool for assessing MXene composites; however, high laser powers and temperatures can lead to the materials' deterioration during the analysis. Therefore, an in-depth understanding of MXene photothermal degradation and changes in its oxidation state is required, but no systematic studies have been reported. The primary aim of this study was to investigate the degradation of the MXene lattice through Raman spectroscopic analysis. Distinct spectral markers were related to structural alterations within the $Ti_3C_2T_x$ material after subjecting it to thermal- and laser-induced degradation. During the degradation process, spectral markers were revealed for several specific steps: a decrease in the number of interlayer water molecules, a decrease in the number of –OH groups, formation of C–C bonds, oxidation of the lattice, and formation of TiO_2 nanoparticles (first anatase, followed by rutile) (Fig. 4). By tracking position shifts and intensity changes for $Ti_3C_2T_x$, the spectral markers that signify the initiation of each step were found. This spectroscopic approach enhances our understanding of the degradation pathways of MXene and facilitates enhanced and dependable integration of these materials into devices for diverse applications, from energy storage to sensors.

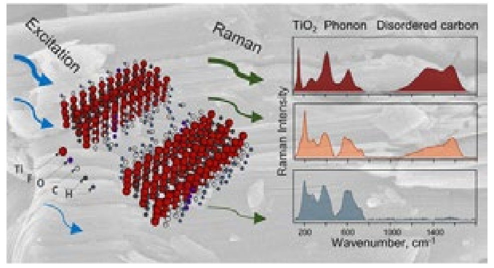

Fig. 4. Illustration of $Ti_3C_2T_x$ MXene evaluation using Raman spectroscopy.

Molecularly imprinted composite-based biosensor for the determination of SARS-CoV-2 nucleocapsid protein

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This article aims to present a comparative study of three polypyrrole-based molecularly imprinted polymer (MIP) systems for the detection of the recombinant severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) nucleocapsid protein (rN). The rN is known for its relatively low propensity to mutate compared to other SARS-CoV-2 antigens. The aforementioned systems include screen-printed carbon electrodes (SPCE) modified with gold nanostructures (MIP1), platinum nanostructures (MIP2), and the unmodified SPCE (MIP3), which was used for control. Pulsed amperometric detection (PAD) was employed as the detection technique, offering the advantage of label-free detection without the need for an additional redox probe. Calibration curves were constructed using the obtained data to evaluate the response of each system. Non-imprinted systems were also tested in parallel to evaluate the contribution of non-specific binding and assess the affinity sensor's efficiency. The analysis of calibration curves revealed that the AuNS-based MIP1 system exhibited the lowest contribution of non-specific binding and displayed a better fit with the chosen fitting model compared to the other systems. Further analysis of this system included determining the limit of detection (LOD) (51.2 ± 2.8 pg/mL), the limit of quantification (LOQ) (153.9 ± 8.3 pg/mL), and a specificity test using a recombinant receptor-binding domain of SARS-CoV-2 spike protein as a control. Based on the results, the AuNS-based MIP1 system demonstrated high specificity and sensitivity for the label-free detection of SARS-CoV-2 nucleocapsid protein. The utilisation of PAD without the need for additional redox probes makes this sensing system convenient and valuable for rapid and accurate virus detection.

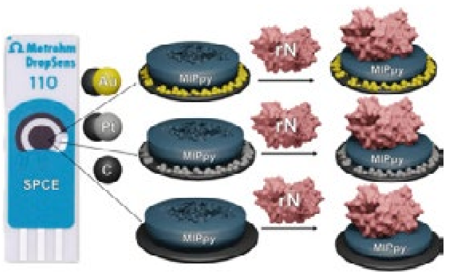

Fig. 5. The scheme represents three types of screen-printed carbon electrode (SPCE) surfaces: unmodified and modified with gold nanostructures or platinum nanostructures.

Molecularly imprinted polypyrrole-based electrochemical melamine sensors

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This study describes the development of a molecularly imprinted polymer (MIP) polypyrrole-based (Ppy-based) electrochemical melamine sensor. Two different modifications of polymeric layers in the design of MIP-based melamine sensor systems were assessed. The addition of gold nanoparticles (AuNPs) or gold(I) complexes in the polymerisation solution containing pyrrole was studied. The characteristics of all polypyrrole layers were evaluated indirectly using a $[Fe(CN)_6]^{3-/4-}$ as a redox probe by application of differential pulse voltammetry (DPV). The most optimal results were obtained when the MIP polymerisation was prepared from a solution containing 50 mM pyrrole, 5 mM melamine, and 0.05 nM 3.5 nm diameter AuNPs. Under these conditions, the observed response of MIP to melamine was 6.61 times greater than that of non-imprinted polymer (NIP). To further characterise the detection of melamine, overoxidised forms of both MIP and NIP were employed. The utilisation of MIP resulted in a linear correlation within the concentration range from 50 nM to 5 µM melamine, with an estimated limit of detection (LOD) of 0.83 nM melamine.

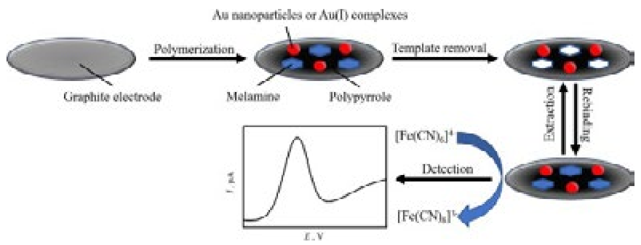

Fig. 6. Schematic representation of molecularly imprinted polypyrrole-based electrochemical melamine sensor development.

Molecular imprinting technology for biomedical applications

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https://doi.org/10.1016/j.biotechadv.2024.108318

Here we present the overview of molecularly imprinted polymers (MIPs) dedicated to biomedical applications and the insights into perspectives of MIPs application in newly emerging areas of biotechnology. Many different protocols applied for MIPs synthesis are presented (Fig. 7). The templates used for molecular imprinting vary from the minor glycosylated glycan-based structures, amino acids, and proteins to whole bacteria. Economic, environmental, rapid preparation, stability, and reproducibility have been highlighted as significant advantages of MIPs. Particularly, some specialised MIPs, in addition to molecular recognition properties, can have high catalytic activity, which in some cases could be compared with other bio-catalytic systems. Therefore, such MIPs belong to the class of so-called "artificial enzymes".

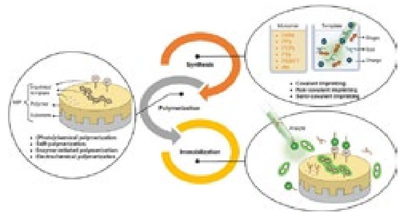
Fig. 7. The most essential stages applied during the formation of molecular imprinted polymers.

Development of an activity-based ratiometric electrochemical switch for direct, real-time sensing of pantetheinase in live cells, blood, and urine samples

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https://doi.org/10.1021/acssensors.4c01658

Pantetheinase is a key biomarker for the diagnosis of acute kidney injury and the monitoring of malaria progression. Currently, existing methods for sensing pantetheinase, also known as Vanin-1, show considerable potential but have certain limitations, including their inability to directly sense analytes in turbid biofluid samples without tedious sample pretreatment. Here, we describe the first activity-based electrochemical probe, VaninLP, for convenient and specific direct targeting of pantetheinase activity in turbid liquid biopsy samples. The probe was designed so that cleavage of the pantetheinase amide linkage, triggered by a self-immolative reaction, simultaneously ejects an amino ferrocene reporter (Fig. 8). Among the distinctive properties of the VaninLP probe for sensing pantetheinase are its high selectivity, sensitivity, enzyme affinity, wide linear concentration range (8–300 ng/mL), and low detection limit (2.47 ng/mL). The designed probe precisely targeted pantetheinase and was free of interference by other electroactive biological species. We further successfully applied the VaninLP probe to monitor and quantify the activity of pantetheinase on the surfaces of HepG2 tumour cells, blood, and urine samples. Our findings indicate that VaninLP holds significant promise as a point-of-care tool for diagnosing early-stage kidney injury, as well as monitoring the progression of malaria.

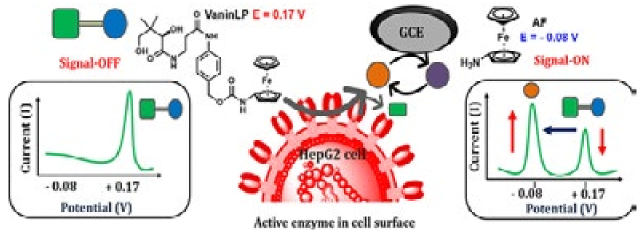

Fig. 8. Schematic illustration of an activity-based ratiometric electrochemical switch for direct, real-time sensing of pantetheinase.

Structural properties of immune complexes formed by viral antigens and specific antibodies shape the inflammatory response of macrophages

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Data on the course of viral infections revealed severe inflammation as a consequence of antiviral immune response. Despite extensive research, there is insufficient data on the role of innate immune cells in promoting inflammation mediated by immune complexes (IC) of viral antigens and their specific antibodies. Recently, we demonstrated that antigens of human polyomaviruses (PyVs) induce an inflammatory response in macrophages. Here, we investigated macrophage activation by IC. We used primary murine macrophages as a cell model, virus-like particles (VLPs) of PyV capsid protein as antigens, and a collection of murine monoclonal antibodies (mAbs) of IgG1, IgG2a, IgG2b subclasses (Fig. 9). The inflammatory response was investigated by analysing inflammatory chemokines and activation of NLRP3 inflammasome. We observed a diverse pattern of chemokine secretion in macrophages treated with different IC compared to VLPs alone. To link the the IC properties with cell activation status, we characterised IC with advanced optical and acoustic techniques. Ellipsometry provided precise real-time kinetics of mAb-antigen interactions, while quartz crystal microbalance measurements showed changes in conformation and viscoelastic properties during IC formation. These results revealed differences in mAb-antigen interaction and mAb binding parameters of the investigated IC. We found that IC-mediated cell activation depends more on IC characteristics, including mAb affinity, than on mAb affinity for the activating Fc receptor. The IC formed by the highest affinity mAb showed a significant enhancement of inflammasome activation. This may explain the hyperinflammation related to viral infection and vaccination. Our findings demonstrate that IC promote the viral antigen-induced inflammatory response depending on antibody properties.

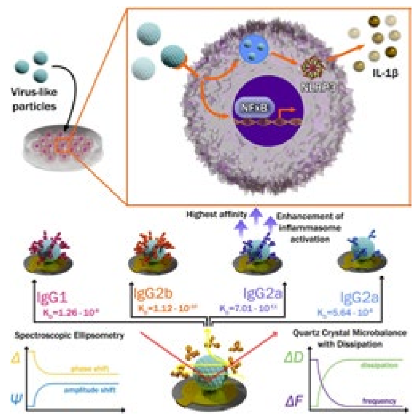
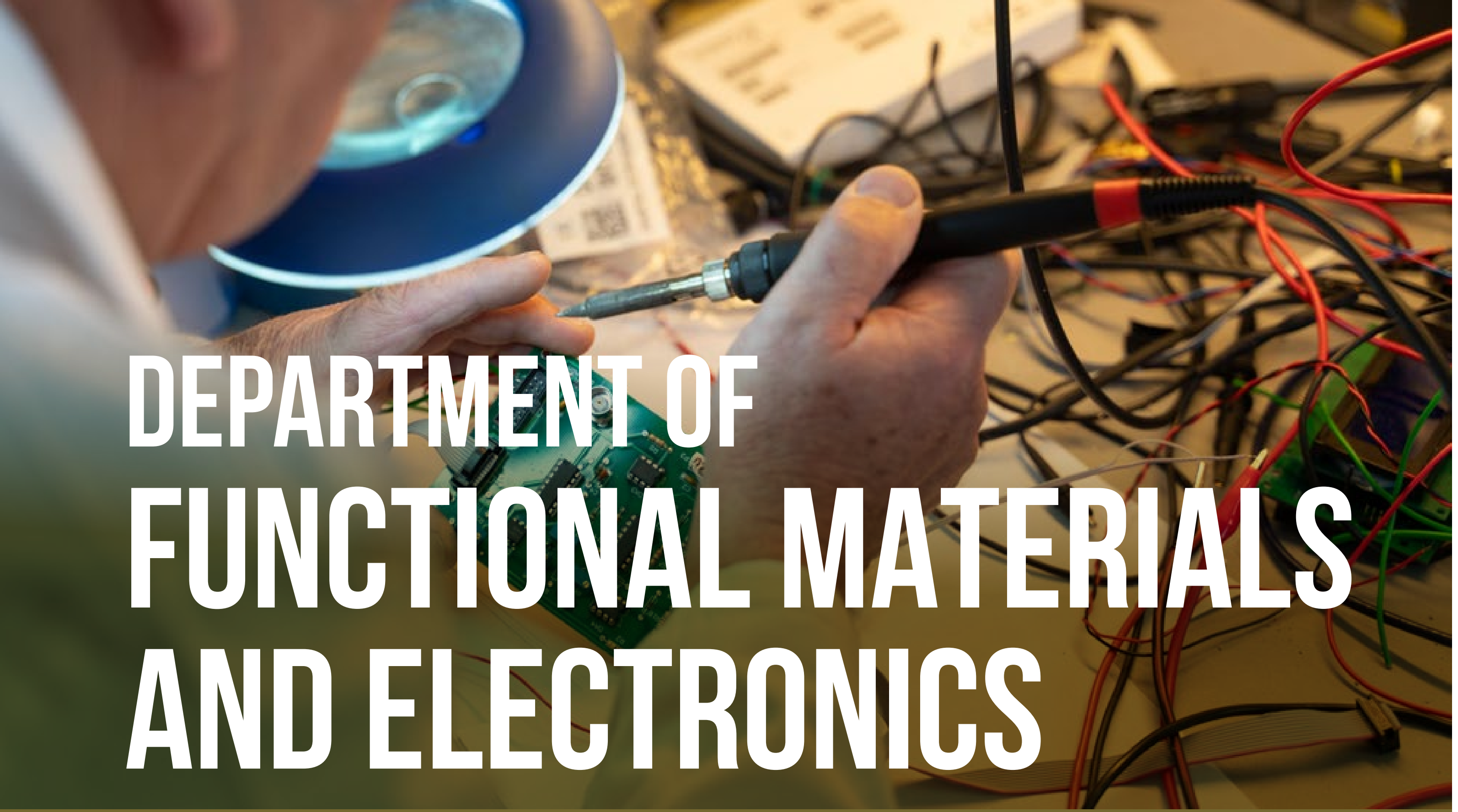


Fig. 9. Graphical summary. Antibodies can enhance viral antigen-induced inflammasome activation in macrophages. NLRP3 inflammasome activation by IC depends on Ab affinity and the amount of Ab covering the surface of the antigen. The SE and QCM-D were used to characterise Ab affinity and real-time formation of IC.



DEPARTMENT OF FUNCTIONAL MATERIALS AND ELECTRONICS

"The investigation of functional materials and their response to electrical, magnetic, optical or biochemical stimuli allows to exploit the material properties for real life applications."

Prof. Dr. Nerija Žurauskienė

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The increasing demand for innovative functional materials with distinctive properties is the driving force of fabrication technologies. Within the Department of Functional Materials and Electronics, significant efforts are being made to develop the technologies of pulsed injection MOCVD, magnetron sputtering, and pulsed laser deposition which are being used to create advanced thin films and nanostructures. Ferromagnetic oxides, Heusler alloys, high-temperature superconductors, and 2D semiconductors, such as graphene, are tailored in our department to be used for different applications. Numerical calculations as well as experimental investigations of specific properties of grown nanostructures are performed to clear up their responses to external stimuli, such as magnetic and electric fields, exposure to light and others, in order to develop spin valves, magnetic field sensors, proximity sensors, biosensors, and other devices.

We are also exploring the impact of electrical pulses on plasma membrane permeability across a variety of cells, from bacteria to mammalian cells. This research focuses on how plasma membrane permeability affects the survival of microorganisms with cell walls and aims to identify specialized testing methodologies. Additionally, there are efforts to develop electroporation-based technologies for managing harmful microorganisms.

Investigations extend to analyzing the effects of short nanosecond electrical pulses on intracellular signals. Concurrently, research is focused on the influence of abiotic factors, such as light, temperature, and electric fields, on cellular signals. This involves using innovative optically transparent polymeric materials for photodynamic therapy and developing organ-on-a-chip devices to explore electrically induced intercellular signals.

Development of photoactive biomaterial using modified fullerene nanoparticles

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doi: 10.3389/fchem.2024.1432624

Medical device-associated biofilm infections continue to pose a significant challenge for public health. These infections arise from biofilm accumulation on the device, hampering the antimicrobial treatment. In response, significant efforts have been made to design functional polymeric devices that possess antimicrobial properties, limiting or preventing biofilm formation. However, until now none of the strategies showed a promissory effect. Thus, antimicrobial photodynamic therapy (aPDT) has been shown as a promising candidate to overcome this problem. Photosensitizers (PS) are the main key component for aPDT and fullerenes have been chosen as PS due to their good quantum yields and lifetimes spans. In this study, polylactic acid (PLA) surface was modified with fullerene (C60) and reaction was proven by XPS analysis. The biopolymer surface was characterized by AFM, SEM, and water contact angle measurements. The obtained results imply that the highest fullerene precipitation was attained when PLA was modified with ethylenediamine (EDA) before the reaction with C60, as the highest carbon increase was identified using XPS following reaction with C60. While samples' hydrophobicity decreased after PLA modification with EDA, it increased after fullerene precipitation. Which implies that bacteria have a lower propensity to attach. Although the surface of the samples became smoother following PLA modification with EDA and reaction with 0.1% C60 precipitation, with 1% C60 precipitation the surface roughness was comparable to unmodified PLA, according to AFM and SEM analyses. Fullerene-based biopolymers could potentially be used in aPDT to make antimicrobial surfaces or medical devices.

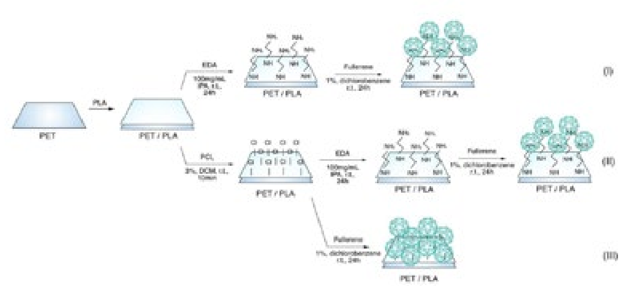

Fig.1. General scheme of Fullerene-based biopolymers synthesis.

Fig.2. (A) PLA, (B) PLA modified with 0.1% fullerene, (C) PLA modified with 1% C60.

Magnetic proximity sensor based on colossal magnetoresistance effect

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https://doi.org/10.1016/j.sna.2024.115518

The development of advanced magnetic proximity sensors (MPS) is crucial for both scientific and industrial applications, where precise measurement of magnetic fields and detection of material properties are essential. In our study we present a novel magnetic proximity sensor (CMR-MPS) leveraging the colossal magnetoresistance (CMR) effect in manganite films, offering significant improvements in sensitivity and versatility. By incorporating both solid and hollow cylindrical permanent magnets (SMC and HMC, respectively), the sensor demonstrates a hyperbolic relationship between the magnetic field response and the distance to ferromagnetic and superconducting targets in static experiments. The dynamic behavior of the sensor, influenced by the magnetization of steel and the induction of eddy currents in duralumin, highlights its potential for detecting and analyzing the motion of various materials. This innovative approach not only enhances the capabilities of magnetic proximity sensors, but also opens new avenues for their application in non-destructive testing and material characterization.

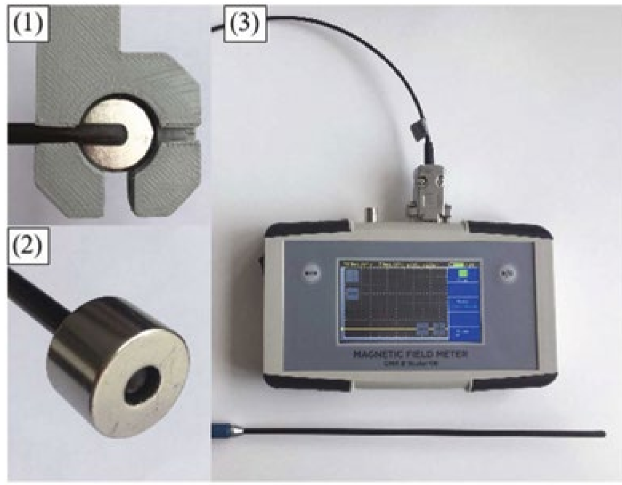

Fig. 3. Magnetic proximity sensor with SMC-design (1) and HMC-design (2). (3) Hand-held meter with CMR-B-scalar probe.

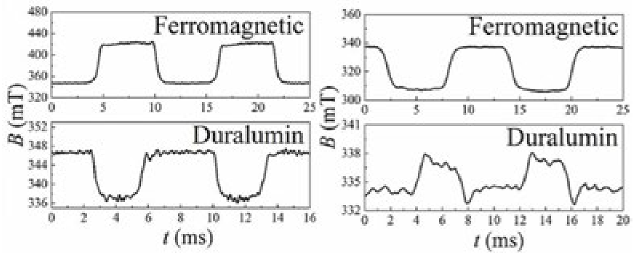

Fig. 4. Dynamic responses of CMR magnetic proximity sensor with SMC (left) and HMC (right) design to the ferromagnetic or duralumin plates at different rotating frequencies.

The advancement and utilization of Marx electric field generator for protein extraction and inducing structural alterations

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Creating innovative electroporation devices is vital for both scientific research and industrial applications. This study presents a two-range, 12-stage Marx pulse generator equipped with thyristor switches, specifically designed for the electroporation of biological cells. The generator utilizes two sets of capacitors (1 μF and 0.25 μF) to produce electrical pulses with varying durations and amplitudes up to 25 kV, providing flexibility for diverse applications.

The generator includes safety features such as overcurrent and overvoltage protection to ensure reliable operation. Testing with resistive loads demonstrated its high output voltage, adjustable repetition rates, and pulse durations. The generator was successfully used for protein extraction from microalgae (Chlorella vulgaris) and for altering the structure of casein micelles (CSMs). The results showed increased membrane permeability, nucleic acid leakage, and protein release in microalgae, as well as changes in particle size and ζ-potential in casein micelles.

These findings highlight the generator's potential for sustainable and environmentally friendly practices in food processing and biotechnology, making it a versatile tool for various applications.

Fig. 5. 12-stage Marx pulse generator.

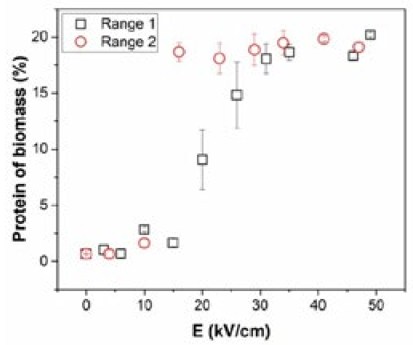

Fig. 6. Extracted protein concentration of *C. vulgaris* after treatment with different electric field strengths.

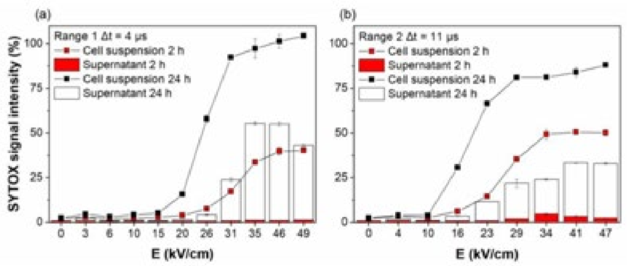

Fig. 7. The SYTOX green fluorescence in microalgae suspension and supernatant after PEF treatment.

Interplay between metal–organic and covalent bonding in single-layer molecular networks

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https://doi.org/10.1039/d4cp01952k

A computational approach for the assembly of metal-organic and covalent single-layer molecular networks on catalytic metal surfaces, using 1,3,6,8-tetrabromopyrene (Br4Py) as prototype molecule, is presented. The proposed coarse-grained lattice model is studied by Monte Carlo simulations. Results indicate that the bonding structure of dehalogenated ensembles is governed by the balance between the metal-coordinated and covalent C-C bonding interactions, the distribution of debrominated species, and the concentration of dissociated (chemisorbed) Br on the surface. Simulations with partially debrominated molecules reveal the assembly of ordered metal-organic phases. Addition of dissociated halogens leads to the formation of many small islands, displaying a short-range order on the Cu and Au surfaces. This suggests that dissociated Br may have an important role in fragmentation of metal–organic networks. Covalent networks formed by completely debrominated molecules are mostly disordered, characterized by short-range glass-like order. Simulations also revealed the growth of molecular arrays with mixed bonding nature, consisting of oligomer chains linked together side-to-side by metal adatoms, as seen in experiments with bromoarenes.

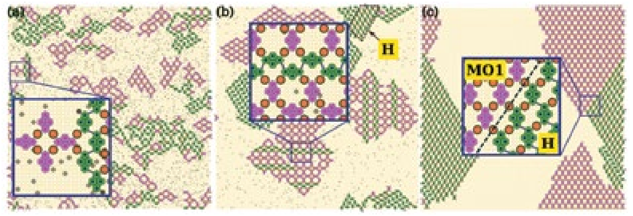

Fig. 8. Coexistence and intermixing of debrominated metal-organic and covalently linked motifs for [dissociated Br]-to-molecule ratios of (a) 3.8, (b) 1, and (c) 0. Color denotations: magenta – molecules restricted to metal-organic bonding; green – molecules with both metal-organic and covalent bonds; gray solid circles represent dissociated Br, and gold solid circles are metal adatoms.

Microphysiological system with integrated sensors to study the effect of pulsed electric field

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https://doi.org/10.1038/s41598-024-69693-w

This study focuses on the use of pulsed electric fields (PEF) in microfluidics for controlled cell studies. The commonly used material for a soft lithography, polydimethylsiloxane (PDMS), does not fully ensure the necessary chemical and mechanical resistance in these systems. Integration of specific analytical measurement setups into microphysiological systems (MPS) are also challenging. We present an off-stoichiometry thiol-ene (OSTE)-based microchip, containing integrated electrodes for PEF and transepithelial electrical resistance (TEER) measurement and the equipment to monitor pH and oxygen concentration in situ. The effectiveness of the MPS was empirically demonstrated through PEF treatment of the C6 cells. The effects of PEF treatment on cell viability and permeability to the fluorescent dye DapI were tested in two modes: stop flow and continuous flow. The maximum permeability was achieved at 1.8 kV/cm with 16 pulses in stop flow mode and 64 pulses per cell in continuous flow mode, without compromising cell viability. Two integrated sensors detected changes in oxygen concentration before and after the PEF treatment, and the pH shifted towards alkalinity following PEF treatment. Therefore, our proof-of-concept technology serves as an MPS for PEF treatment of mammalian cells, enabling *in situ* physiological monitoring.

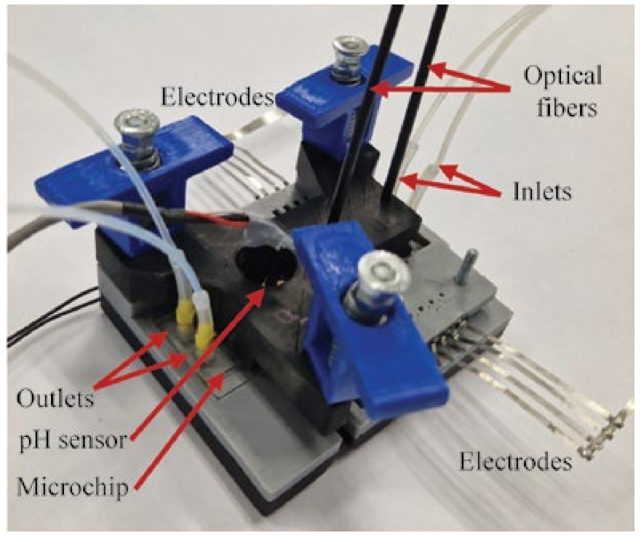

Fig. 9. The prototype of MPS.

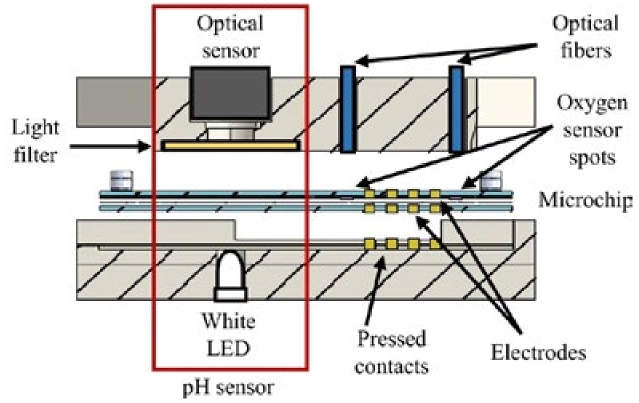

Fig. 10. Cross-section and decomposition of the supporting jig.

RF power saving system for smart homes

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https://doi.org/10.1016/j.heliyon.2024.e39862

Here we present the results of harvesting the RF energy of a 2.4 GHz Wi-Fi signal for supply of smart home leak sensors network. The collected RF energy has been used as an additional source to power the sensors. The aim was to determine the limiting values of the RF signal source power and the limiting distances between the RF energy harvesting system and the RF signal source, i. e. the values which enable harvesting the RF energy and charge the energy storage capacitor. Therefore, the PCB-based Yagi-Uda type antenna for receiving RF signal and a suitable RF energy harvesting system was designed.

The hardware model of the harvesting system was studied using this antenna, as well as other antennas using a signal generator and Wi-Fi router as sources of RF signal. The obtained results demonstrate that at typical Wi-Fi router transmitting power (10–17 dBm) the RF energy can be collected when the router is several tens of centimetres away from the harvesting antenna. When the router with a maximum allowed power of 20dBm is used, the distance allowing to collect the RF energy reaches 120 cm, but only if transmitting and receiving antennas are both of the Yagi-Uda type.

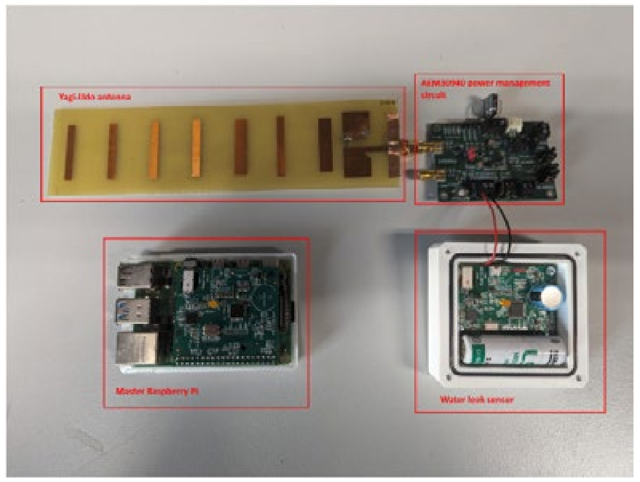
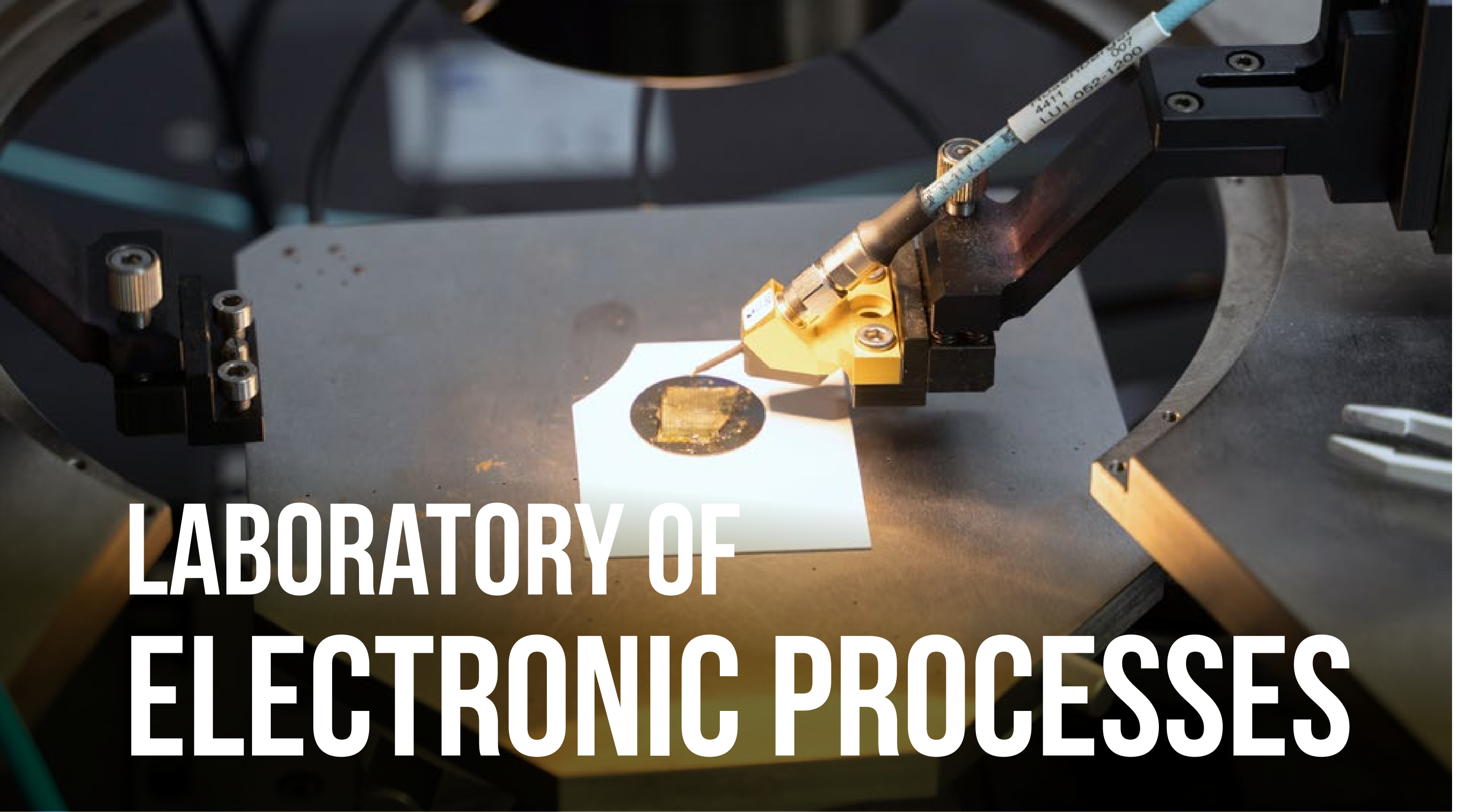


Fig. 11. Water leak sensor with the RF energy harvesting system and master of the sensor network based on the Raspberry PI.



LABORATORY OF ELECTRONIC PROCESSES

„The greatest asset and proudest achievement of our Laboratory is the professional expertise of our researchers.“

Dr. Jonas Gradauskas

Head of Laboratory, Senior Researcher

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The mission of the Laboratory is to conduct high-level fundamental and applied research aimed to elevate global reputation of our country through scientific excellence. Our goal is to advance fundamental and applied scientific research in the field of charge carrier transport and electronic processes associated with electromagnetic radiation ranging from terahertz frequencies to visible light. The activities of research and experimental development of the laboratory are focused on:

- investigation of the interaction of electromagnetic radiation with semiconductor nanostructures across a broad frequency spectrum;
- study of optical transitions in semiconductor nanostructures using highly sensitive single-photon detection equipment;
- solving Maxwell's equations in waveguide microwave systems and metamaterials;
- development of methods for desynchronisation and damping of interacting oscillator arrays;
- research on charge carrier transport in perovskite and inorganic semiconductor solar cells, including hot carrier phenomena;
- development of new innovative devices for microwave, terahertz, and infrared electronics.

Some aspects of hot carrier photocurrent across GaAs p-n junction

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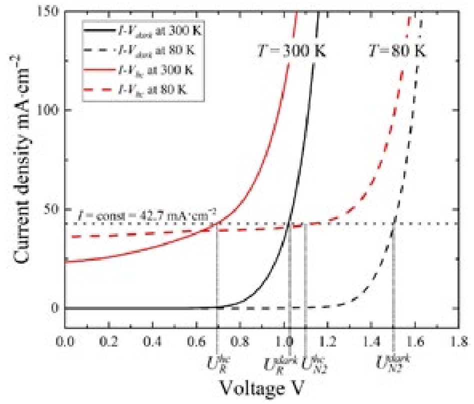
https://doi.org/10.3390/inorganics12060174

Hot carriers are suspected as an additional intrinsic “pre-thermalisation loss” preventing realised solar cells from reaching the theoretical Shockley-Queisser limit. Based on the temperature coefficient of the I-V characteristics, we propose a novel technique for estimating the hot carrier temperature of a p-n junction. The calculation results fall within the reasonable range of carrier temperatures obtained by other methods.

Fig. 1. I-V characteristics of the p-n structure in the dark (black) and with hot carrier photocurrent (red) at 300 K (solid lines) and 80 K (dashed lines) temperature. The data of the I-Vs was used to calculate the hot carrier temperature.



Semiconductor nanowire metamaterial for tuneable enhanced absorption

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https://doi.org/10.1007/s13538-024-01570-3

The development of a semiconductor adjustable absorber in the THz opens up new possibilities for quantum information science, imaging, health, and sensing applications. Here, we build a unique semiconductor ellipse-shaped nanowire matrix that exhibits increased absorption in the 1 to 3 THz region. The maximum absorption efficiency is reached by adjusting the dimensions of the major and minor axes of the ellipse, the distance between the nanowires and the temperature of the metamaterial. In addition, it is shown that varying of magnetic fields gives almost constant absorption values.

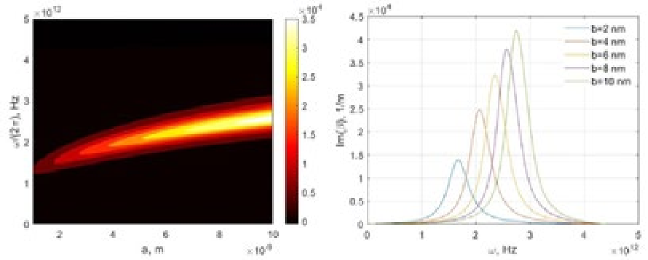

Fig. 2. Simulations of the absorption for ellipsoidal nanowires as a function of frequency and dimensions at: (a) fixed b = 4 nm and (b) fixed a = 5 nm. The distance between the nanowires S = 60 nm and the temperature T = 350 K. Here, a is the length of the semi-major axis, and b is the length of the semi-minor axis.

Microwave bow-tie diodes on bases of 2D semiconductor structures

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https://doi.org/10.3390/cryst14080720

Planar microwave bow-tie diodes on the base of selectively doped semiconductor structures are successfully used in the detection and imaging of electromagnetic radiation in millimetre and submillimetre wavelength ranges. A comprehensive study of a series of planar bow-tie diodes, from a simple asymmetrically shaped submicrometre-thick n-GaAs layer to diodes based on various selectively doped GaAs/AlGaAs structures positioned on a semi-insulating substrate or an elastic dielectric polyimide film, was carried out. The diodes were investigated using DC and high-frequency probe stations, both in the dark and under white light illumination, allowing sufficient data for statistical analysis of the electrical parameters to be obtained. Our investigation revealed that _detection properties of the bow-tie diodes are strongly determined by the energy states residing in semiconductor bulk, surface, and interfaces.

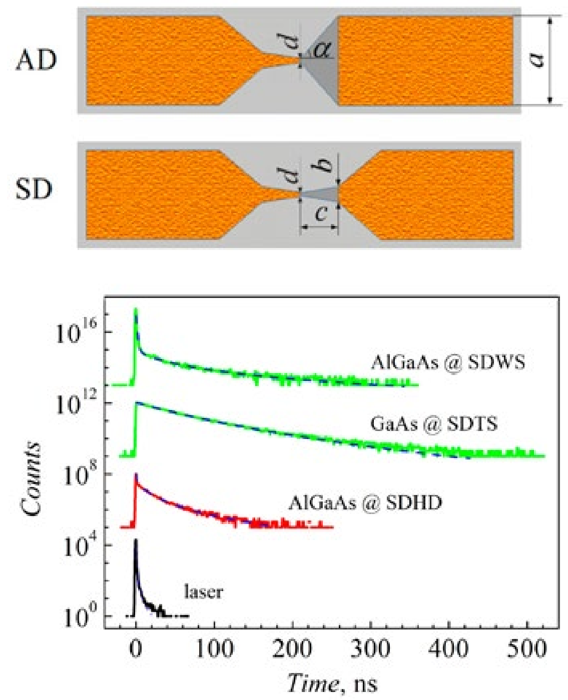
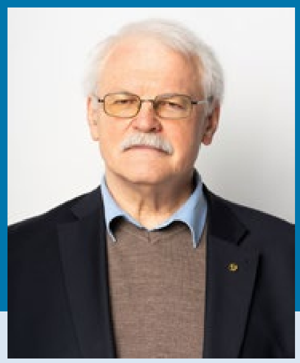


Fig. 3. (a) Schematic top-view of asymmetric (AD) and symmetric (SD) bow-tie microwave diodes. (b) Time-resolved photoluminescence spectra of three different selectively doped layered structures used for fabrication of the diodes.

DEPARTMENT OF FUNDAMENTAL RESEARCH



„Without fundamental science, there is no Science...."

Prof. Dr. Vladas Vansevičius
Head of Department, Principal Researcher
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The main goal of the department is to produce high-level scientific knowledge for increasing the country's competitiveness in the long-term perspective. Our research focuses on developing and improving theoretical and experimental methods for solving fundamental problems in biophysics, solid state physics, optics, and astrophysics.

Current research directions of the department:

- Application of nonlinear dynamics and control theory methods in the study of complex neural network systems.
- Development of electronic structure theory methods for studying optoelectronic phenomena in semiconductors.
- Development and application of fluctuation methods to study wide-bandgap semiconductors.
- Engineering of vector optical fields: generation and study of the behaviour of photonic systems.
- Studies of the evolution of the universe from our Galaxy to the Big Bang.

Subaru Suprime-Cam wide-field BVI stellar photometry of the M33 galaxy

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We have surveyed the disk of the M33 galaxy in the Local Group. CCD images in the BVI-passbands were obtained with the Subaru Telescope equipped with the Suprime-Cam mosaic camera. The photometry catalogue of 803 095 stars was published. We determined the M33 distance of 843 kpc using the tip of the red giant branch technique. We found young (<100 Myr) stellar populations up to the radius of 10 kpc. The youngest stars (<15 Myr) reside up to the radius of 8 kpc. This distribution of stellar populations suggests an outside-in scenario of recent star formation in the disk of M33.

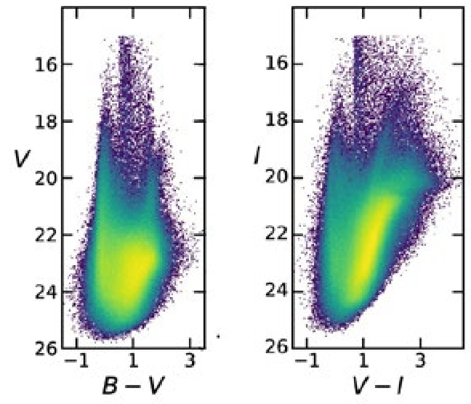

Fig. 1. Photometry results of stars from our M33 survey.

Limitations of aperture photometry for star cluster studies

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https://doi.org/10.1051/0004-6361/202449680

The aim of our study was to determine the best achievable limits on the accuracy and applicability of the aperture photometry method for studying star clusters in the Local Universe. We computed a large network of artificial 3D star clusters spanning the parameter space of the M31 clusters. To determine the applicability of aperture photometry to star cluster studies, we measured the simulated images and performed parameter determination tests. We showed that cluster colours have to be measured using apertures larger than the clusters' half-light radii. Also, we demonstrated that the parameter determination of young clusters (~10 Myr) is a difficult problem regardless of the aperture size used. Therefore, it is advisable to determine the parameters of these clusters using colour-magnitude diagram fitting methods.

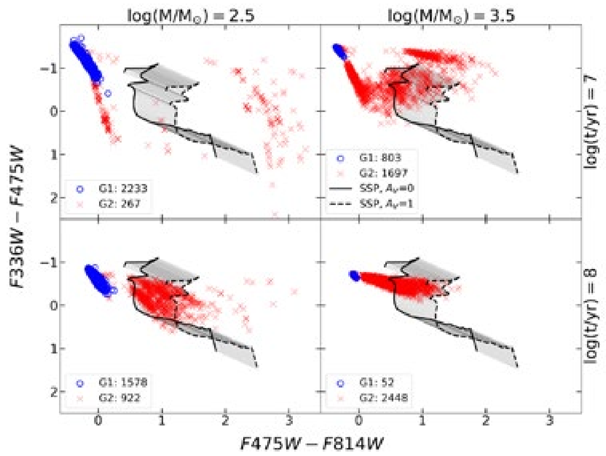

Fig. 2. Two colour diagrams of simulated stochastic star clusters. Each panel shows aperture photometry results for different combinations of cluster mass (marked above the panels) and age (marked to the right of the panels). Shaded areas mark non-stochastic solar metallicity models from 10 Myr to 12.6 Gyr.

Effects of the last activity episode in our Galaxy

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Submitted to Astronomy and Astrophysics

Our Galaxy contains two vast bubbles of extremely hot plasma rising from the centre perpendicularly to the disc. These so-called Fermi bubbles are surrounded by shells of denser, but still hot, gas expanding with a velocity of several hundred km/s. We developed a model that successfully explains these observations. The model relies on the theory of galactic outflows driven by active galactic nuclei, which has been used to explain large-scale outflows in many other galaxies. In our Galaxy, the activity in the nucleus happened 6 million years ago and lasted about a million years. After it ended, the outflow continued to expand due to its high pressure. Our hydrodynamical simulation reproduces the size and shape of the inner hot bubbles and their surrounding shells, as well as the velocity of approaching and receding gas.

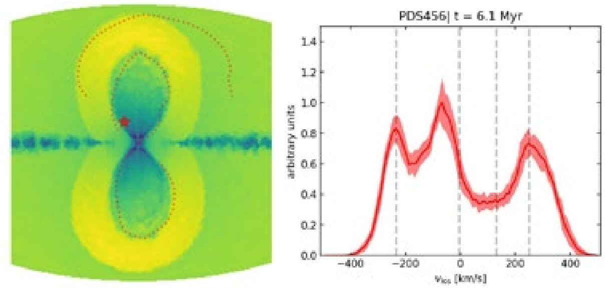

Fig. 3. Left: Gas density integrated along the line of sight in our hydrodynamical simulation; brighter colours represent higher density. Red dotted lines show the contours of the observed Fermi bubbles (inner) and the surrounding shell (outer). Red star marks the coordinates of quasar PDS 456 which has been used to measure gas velocities. Right: histogram of radial gas velocities in the direction of the quasar. Vertical dashed lines show the velocities of the main observed absorption features in the quasar's spectrum.

Star formation enhancement by galactic outflows

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https://doi.org/10.1051/0004-6361/202450286

Large-scale outflows driven by active galactic nuclei (AGN) move much faster than typical gas flows in galaxies, have much higher temperature and, consequently, pressure. Usually, it is thought that any gas clouds encountering an outflow get shocked and dispersed very quickly. However, using hydrodynamical simulations, we showed that under certain conditions – mostly outflow velocities below 200 km/s and temperatures above 10 thousand Kelvin – the clouds are compressed instead. This leads to faster fragmentation and star formation and can explain the observations of stars forming within AGN-driven outflows.

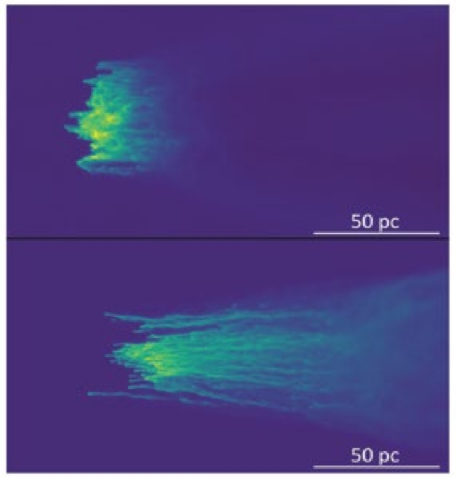

Fig. 4. Top: a 10 thousand Kelvin outflow, moving from left to right at 60 km/s, gently compressed a 100 thousand Solar mass gas cloud and spurs its fragmentation. Bottom: same as above, but the outflow velocity is 200 km/s.

Quintessence in the Weyl-Gauss-Bonnet model

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https://doi.org/10.1088/1475-7516/2024/02/040

The accelerated expansion of the Universe remains among the biggest puzzles in cosmology. One plausible explanation for the acceleration could be the failure of General Relativity to accurately describe Nature at the largest distance scales. We explore such a possibility within the framework of Gauss-Bonnet Gravity (GBG) models, which can be motivated by theories of quantum gravity. These models allow for the apparent violation of the weak energy condition without the usually associated instabilities. Tentative hints of such a violation are observed in the expansion of the Universe. In this work we generalise GBG models by allowing for two geometric structures, the metric and the connection, to be independent fields, and study the evolution using dynamical systems analysis. However, we find that it is difficult to reproduce the known history of the Universe and simultaneously satisfy observational constraints on the speed of gravitational waves.

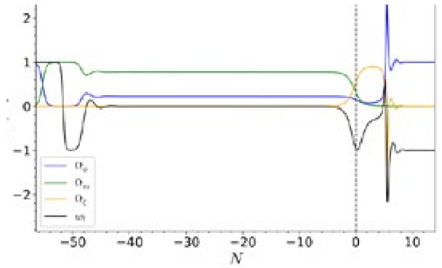

Fig. 5. Evolution of cosmological parameters for one realisation of the model.

Application of next-generation reservoir computing for predicting chaotic systems from partial observations

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Next-generation (NG) reservoir computing (RC) is a machine learning approach that has been recently proposed as an effective method for predicting the dynamics of chaotic systems. A conventional RC processes information signals using the nonlinear responses of a multidimensional dynamic system known as a reservoir. In RC, the weights connecting the input layer to the reservoir and the recurrent connection weights are assigned randomly and remain fixed. Only the readout weights are trained using a simple and efficient least squares method. The NG-RC modification avoids the random nature inherent in traditional RC and requires fewer meta-parameters. It uses a nonlinear vector autoregression (NVAR) algorithm with a feature vector consisting of several time-delayed input signals and their nonlinear functions, which are usually taken in polynomial form. Here we study the effectiveness of the NG-RC method when only a scalar time series are available for observation. The prediction of time series of chaotic Rössler and Lorenz systems, as well as chaotic electronic circuit, has been considered. We found that prediction is only effective if the feature vector of a NVAR algorithm contains monomials of sufficiently high degree. In addition, we proposed a more efficient NG-RC-Ch algorithm in which monomials are replaced by Chebyshev polynomials. The Fig. 6 demonstrates that the prediction time of NG-RC-Ch is approximately two Lyapunov time units longer than that of NG-RC.

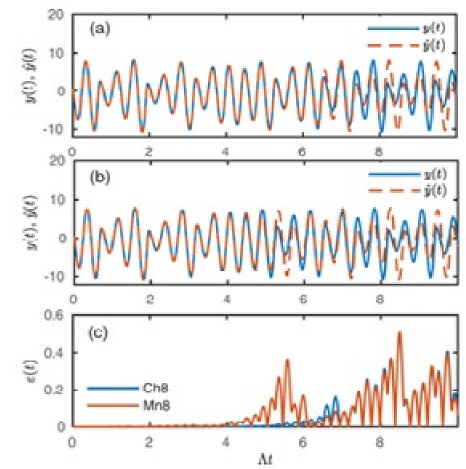

Fig. 6. Comparing NG-RC-Ch and NG-RC algorithms using Chebyshev polynomials and monomials of degree m = 8 for the Rössler system. The blue continuous curves in top and central panels show the original time series *y(t)*. The time series predicted by the NG-RC-Ch (top) and NG-RC (central) algorithms are shown by the red dashed curves. The blue and red curves in bottom panel show the absolute errors for the NG-RC-Ch and NG-RC algorithms, respectively. The time is normalized by the largest Lyapunov exponent.

Constraining the general oscillatory inflaton potential with freeze-in dark matter and gravitational waves

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https://doi.org/10.1088/1475-7516/2024/08/051

In this work we investigate how the determination of Dark Matter (DM) interaction cross section by particle physics experiments could be combined with astronomical measurements of Gravitational Waves (GWs) to constrain the physics of the very early Universe. If DM is produced by the freeze-in mechanism, its abundance is very sensitive to the details of the early Universe physics. On the other hand, for certain evolution scenarios of the Universe, the GWs generated by quantum fluctuations during cosmic inflation are amplified up to the detectable level by future observatories. We show how combining the two measurements in this scenario we gain a new method to determine the energy scale of inflation. Determination of this energy scale is the key to really understand the origins of the Universe.

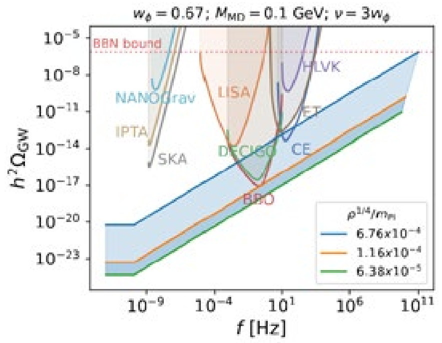

Fig. 7. An example of the range of GW spectra for one set of cosmological parameters. Sensitivity curves of various GW observatories are also shown.

Optical lineshapes for orbital singlet to doublet transitions in a dynamical Jahn-Teller system: The NiV⁻ centre in diamond

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https://doi.org/10.1103/PhysRevB.110.075303

We are modelling the systems dominated by Jahn-Teller (JT) interactions, which frequently occur in crystal defects. By applying a novel first-principles multimode dynamical JT approach, we successfully captured the complex optical lineshape of the negatively charged nickel vacancy centre in diamond, a system characterized by a substantial JT effect. This study highlights the critical role of JT-active modes in affecting optical lineshapes and demonstrates the power of advanced techniques for modelling optical properties in complex systems with multiple JT-active frequencies.

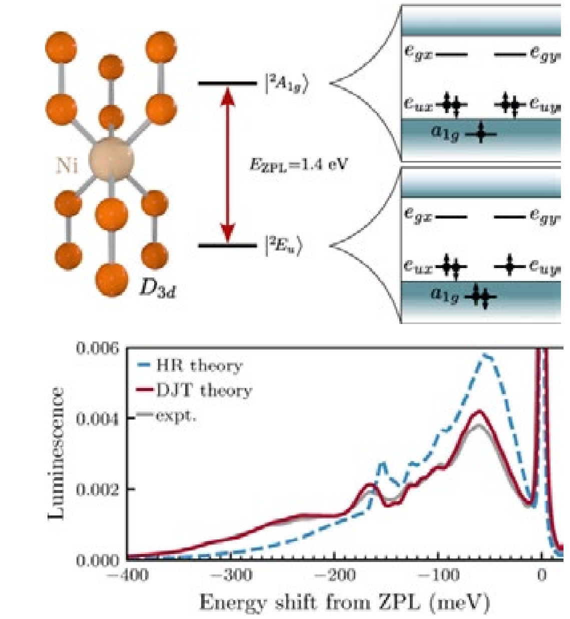

Fig. 8. Theoretical model of the nickel-vacancy (NiV–) centre in diamond and luminescence lineshapes.

Blue quantum emitter in hexagonal boron nitride and a carbon chain tetramer

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https://doi.org/10.1021/acsanm.4c02722

In this work, we performed *ab initio* modelling of a carbon chain tetramer in hexagonal boron nitride (h-BN). We found excellent agreement between its calculated optical properties and the experimental characteristics of the blue quantum emitter, known as the B-centre. The calculated zero-phonon line (ZPL) energy of 3.13 eV closely matches the experimental value of 2.85 eV, and the predicted radiative lifetime of 1.62 ns aligns well with the observed range of 1.8–2.1 ns. Our analysis also indicates weak electron-phonon coupling (S = 1.59) and a Debye-Waller factor (DWF) of 0.25, consistent with the experimental value of 0.26. Additionally, we found no significant linear Stark shift of the ZPL for both in-plane and out-of-plane external fields, which agrees well with the experimental results.

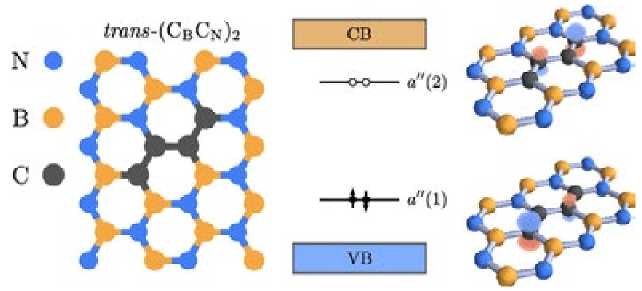
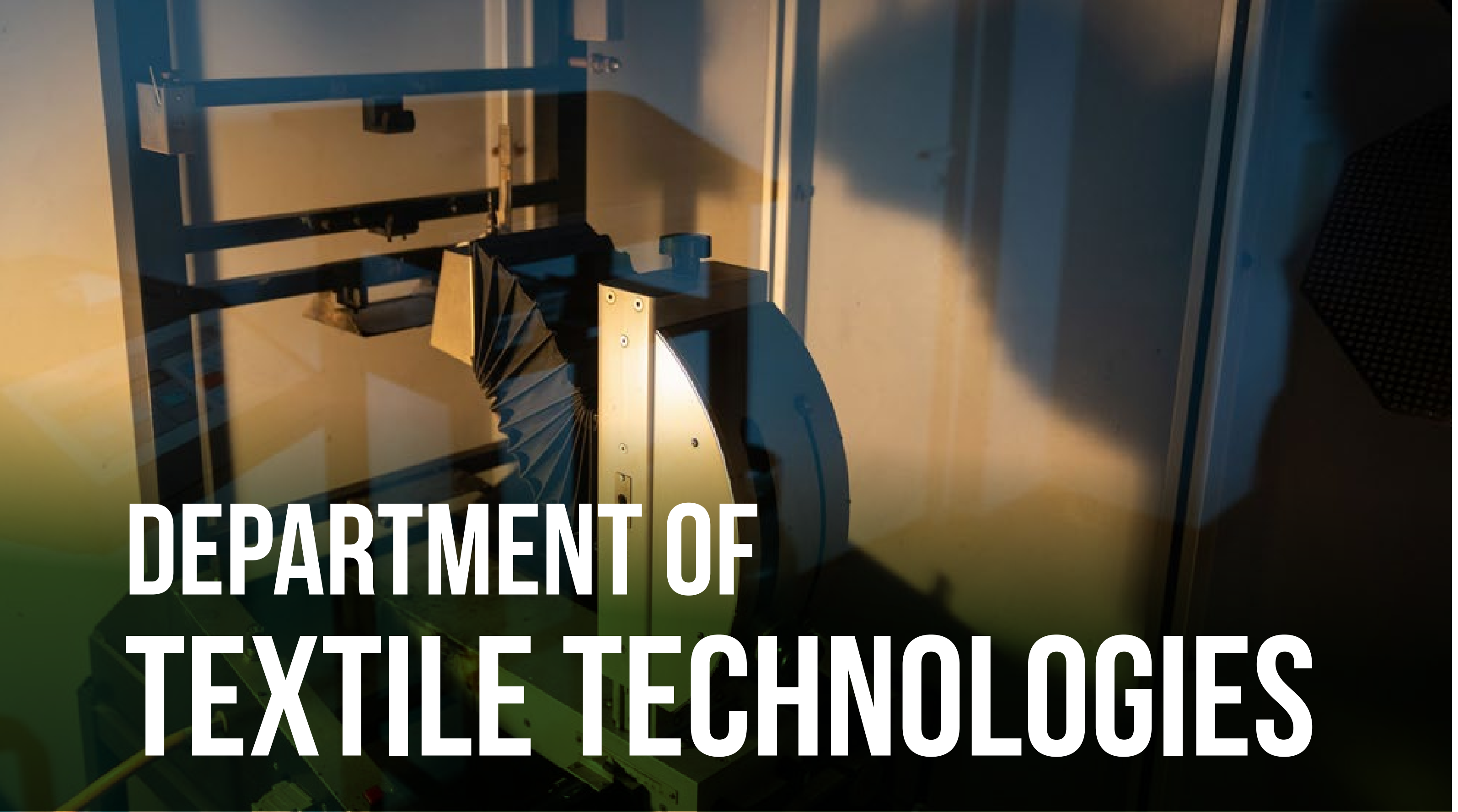


Fig. 9. *Cis* and *trans* configurations of the carbon chain tetramer $(C_BC_N)_2$ in h-BN.



DEPARTMENT OF TEXTILE TECHNOLOGIES

„Driven by innovation and sustainability, the Department of Textile Technologies develops advanced textile solutions for both the civilian and defence sectors, specializing in eco-efficient processes and protective fabric technologies".

Dr. Julija Baltušnikaitė-Guzaitienė

Head of Department, Senior Researcher
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The Department of Textile Technologies remains at the forefront of innovation, offering sustainable and high-performance textile solutions. This year, we prioritized the development of energy-efficient finishing processes to reduce environmental impact, reflecting our commitment to eco-friendly practices in textile manufacturing. Our research integrates advanced technologies to create functional textiles that are not only sustainable but also responsive to modern industry demands. In parallel, our department has made significant strides in military textile projects, with a continued focus on adaptive camouflage systems and protective fabrics for defence applications. Supported by the European Defence Fund, these projects aim to enhance soldier survivability through textiles that adapt to diverse environmental conditions and ensure ballistic and thermal protection.

In addition to product innovation, we provide a comprehensive range of services, including material testing in accredited laboratories, certification of protective clothing, and quality assessment of textiles. Capabilities of our department in testing and certification of personal protective equipment are integral to maintain the highest standards of quality and safety, enabling industries across Europe to comply with regulatory requirements.

Through interdisciplinary research and close collaboration with industry partners, we strive to push the boundaries of textile technology. Our goal is to deliver innovative products that meet the highest standards of quality, safety, and sustainability, contributing to both civilian and defence sectors. As we move forward, our department remains dedicated to advancing textile innovations that address the complex challenges posed by a rapidly changing world.

Electro-magnetic shielding textiles with conductive organic polymeric coating

European Unitary Patent No. EP 3854933 "Manufacture of Electro-Magnetic Shielding Textiles with Conductive Organic Polymeric Coating" by Dr. A. Abraitienė, Dr. A. Sankauskaitė, and Dr. V. Rubežienė

The most significant outcome of the Department's research and development activities in 2024 is the European Unitary Patent No. EP 3854933B1, titled Manufacture of Electro-Magnetic Shielding Textiles with Conductive Organic Polymeric Coating. This invention relates to the development of water-wash-resistant, electrically conductive, wearable woven textiles. These materials are coated with formulations containing an intrinsically conductive polymer (ICP) complex, specifically poly (3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS), as the conductive component (Fig. 1). The primary purpose of the invention is to provide effective shielding against non-ionizing electromagnetic radiation (EMR) within frequency ranges identified as potentially hazardous to human health. The research involved the application of PEDOT:PSS to woven fabrics derived from wool, polyamide, cotton, and their respective blends (Fig. 2). The aim of the invention also is to create a water-wash resistant conductive crosslinked PEDOT:PSS film on the above mentioned woven textile materials to improve the resistance performance of coated fabrics. The present invention is partly based on the idea of electrostatic interaction of the water soluble conjugated polyelectrolyte PEDOT:PSS negatively charged sulfonate counter ions with protonated amino groups in the wool and amide bonds in the polyamide as well as positively charged sites of chemically modified cotton. This invention is also based on a non - dispersible and non-delaminable conductive polymeric coating of textile material formation through PEDOT:PSS and divinylsulfone (DVS) physical crosslinking which can cause a coagulation of conductive polymer dispersion and decrease its water solubility but does not affect its electrical conductivity.

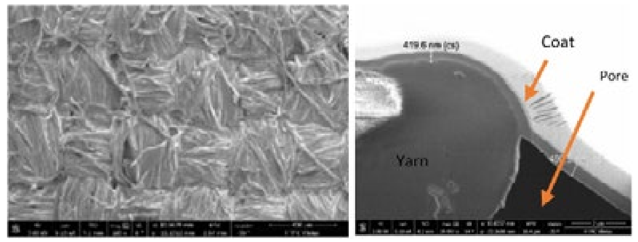

Fig.1. PEDOT:PSS coated fabric.

Fig. 2. PEDOT:PSS coated fabric:
a) initial, b) with PEDOT:PSS coating.

Investigation of salt-added polyethylene oxide/chitosan nanofibers production

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https://doi.org/10.3390/ma17010132

The distinctive amphiphilic nature and unique mechanical attributes of polyethylene oxide (PEO) leads to a successful electrospinning of chitosan (CS) blends with PEO into nanofibers. The addition of salt (NaCl) changes the behaviour of polymer macromolecules: at lower concentrations of salt, the chitosan chains experience increased stretching and dispersion due to electrostatic repulsion. This phenomenon enables the formation of flexible PEO chains to readily formed molecular complexes through hydrogen bonding with chitosan. Our study examined the impact of salt concentrations in PEO on the spinnability of CS/(PEO+NaCl) blends. It was found that the addition of salt reduced the viscosity and improved the conductivity of the solutions and processed fiber mats. However, the spinning process was complicated because of the wet fibers reaching the collector. SEM images (Fig. 3) revealed undissolved salt crystals in spun fiber mats. Software analysis of nanofiber orientation and diameter revealed the results consistent with microscopic measurements, showing diameter discrepancies ranging from 0% to 12%. Sodium chloride significantly enhanced the electrical properties increasing the conductivity of PEO solutions by over 50 times and CS/PEO blends by 6 times compared to salt-free solutions. Fourier-transform infrared spectroscopy (FTIR) analysis indicated no significant changes in the chemical composition due to variations in polymer concentration or salt addition. The analysis of Differential Scanning Calorimetry (DSC) revealed semicrystalline structures in all manufactured CS/(PEO+NaCl) blend nanofibers.

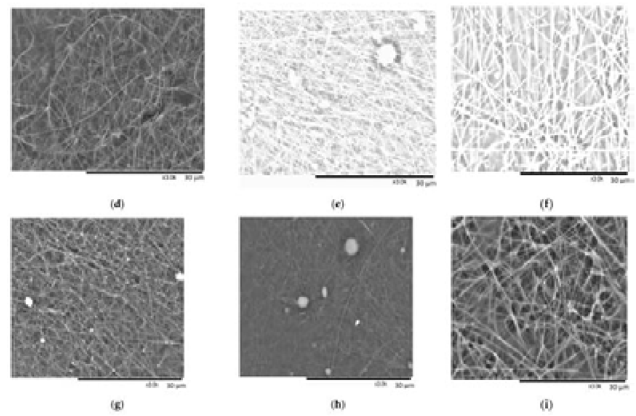

Fig. 3. Segmented SEM images for determination of fiber diameter distribution with ImageJ:
(a) PEO10 NaCl; (b) PEO15 NaCl;
(c) PEO20 NaCl; (d) CS90 + PEO10 NaCl; (e) CS90 + PEO15 NaCl;
(f) CS90 + PEO20 NaCl; (g) CS50 + PEO10 NaCl;
(h) CS50 + PEO15 NaCl; (i) CS50 + PEO20 NaCl.

NATIONAL METROLOGY INSTITUTE

„Without metrology there is no measurement, without measurement, there is no knowledge. Accurate measurements build great trust."

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Metrology: The Science of Accurate and Reliable Measurement

Metrology is the science of measurement, playing a crucial role in ensuring accuracy, reliability, and consistency across various fields—from scientific research and industry to healthcare and trade. At its core, metrology is not just about obtaining measurement results but also about validating their correctness and defining their limitations. By assessing uncertainty and maintaining traceability, metrology provides the foundation for confidence in data, supporting innovation, quality assurance, and global standardization.

FTMC has been authorized to perform and implement the functions of the National Metrology Institute (NMI) since July 1, 2014. To ensure compliance with international standards, a Quality Management System (QMS) was established in accordance with LST EN ISO/IEC 17025:2018. The QMS undergoes regular peer reviews and has been recognized by EURAMET. In 2021, the NMI of Lithuania became one of the eight NMIs from the Nordic-Baltic region to establish the European Metrology Network (EMN) *"Smart Specialisation in Northern Europe"*. In 2023, FTMC further expanded its engagement by joining the European Metrology Network for Pollution Monitoring.

Currently, FTMC maintains the national standards in the seven areas of measurements: electricity and magnetism, ionising radiation, length, mass, amount of substance, 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 -195oC to +961,78o C) is of the primary level, while the reference point of the freezing point of Cu (+1084,62 oC) is of the secondary level.

The main challenge in chemical metrology is that its fundamental SI unit, the mole, cannot be directly realized in practice. Instead, measurements typically focus on substance concentration rather than absolute quantity. Chemical metrology involves the measurement of composition, concentration, and purity of substances, often within complex matrices. Unlike physical measurements, chemical measurements are influenced by factors such as sample preparation, matrix effects, and chemical interactions, making them more challenging to standardize and obtain reliable results. Ensuring metrological traceability and accuracy in chemical measurements requires the use of certified reference materials, validated methods, and rigorous uncertainty evaluation.

The reliable, traceable and accurate chemical measurements in different sectors of biotechnology, healthcare, safety and environment protection are provided by the staff of the **Laboratory for Reference Materials and Measurements (LRMM)**. 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 the NMI is responsible for ionizing radiation measurements, including the absolute activity of radionuclides using primary and secondary methods. Beta-emitters such as ^{3}H, $^{1}4C$, ^{36}Cl, ^{63}Ni, ^{90}Sr, $9^{9}Tc$, and ^{129}I are standardized using the TDCR instrument, achieving a standard uncertainty of 0.3 – 0.6% (k = 1). Meanwhile, radionuclides like ^{18}F, ^{60}Co, ^{67}Ga, ^{99}mTc, ^{111}In, ^{131}I, ^{137}Cs, ^{153}Sm, ^{177}Lu, ^{201}Tl, and ^{223}Ra are standardized using well-type dose calibrators, with a standard uncertainty of 1.0 – 2.2% (k = 1). The laboratory also conducts calibrations of radiation sources, spectrometers, and dose calibrators, while performing research on radionuclide dispersion, radioactive waste composition, and sample analysis. The calibrations and sample measurements, ensuring traceability to the National Standard of radionuclide activity, have been carried out for Lithuanian hospitals and other customers.

Both the national standard of mass and the national standard of length were transferred to FTMC by the Government Decision of the Republic of Lithuania in 2019.

The Length Unit Standard Laboratory (LUSL) is responsible for the field of length. Main objectives are

- calibration of gauge block measurement value from 0.5 mm to 100 mm with expanded uncertainty Q [48 nm,
- 0.9·10-6 L] nm;
- calibration of gauge block comparators with expanded uncertainty of 0.03 mm;
- calibration of micrometers (measurement range (0-100) mm) with expanded uncertainty of 3.6 mm;
- calibration of calipers (measurement range (0-1000) mm) with expanded uncertainty Q [60 mm, 10·10-6 L] nm;
- calibration of dial gauge (measurement range (0-50) mm, resolution 0.01 mm) with expanded uncertainty Q [7 mm, 7·10-6 L] mm;
- calibration of dial gauge (measurement range (0-50) mm, resolution 0.001 mm and 0.002 mm) with expanded uncertainty of 0.7 mm and 1.2 mm, respectively.

The **Mass Unit Standard Laboratory (MUSL)** The accuracy of mass measurements is crucial in trade, legal metrology, and scientific research, highlighting the importance of continuous advancements in mass metrology. The primary standard for mass, historically based on the International Prototype of the Kilogram (IPK), has transitioned to a definition based on the Planck's constant in 2019, ensuring long-term stability and reproducibility.

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.

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