ISSN 2669-1930 (online)

26TH INTERNATIONAL CONFERENCE-SCHOOL

WHEN
26–30 August 2024

WHERE
Palanga Lithuania

ADVANCED MATERIALS AND TECHNOLOGIES

2024

BOOK OF ABSTRACTS

ISSN 2669-1930 (online)

Book of Abstracts
of 26th International Conference-School

ADVANCED MATERIALS AND TECHNOLOGIES

26-30 August 2024, Palanga, Lithuania

Kaunas, 2024

Organizers:
Institute of Materials Science of Kaunas University of Technology (KTU)
Lithuanian Materials Research Society (LT-MRS)
Vilnius University (VU)
University of Latvia (LU)
Riga Technical University (RTU)
University of Tartu (TU)
Center for Physical Sciences and Technology (FTMC)
University of Southern Denmark (SDU)
Applied Research Institute for Prospective Technologies (ProTech)

Programme committee:
Prof. S. Tamulevičius (KTU) – *chairman*
Prof. K. Baltakys (KTU)
Prof. J. V. Gražulevičius (KTU)
Prof. A. Kareiva (VU)
Prof. G. Juzeliūnas (VU)
Prof. G. Tamulaitis (VU)
Dr. M. Mackoit Sinkevičienė (VU)
Dr. R. Butkutė (FTMC)
Prof. D. Erts (LU)
Prof. Y. Dekhtyar (RTU)
Prof. H.-G. Rubahn (SDU)
Dr. R. Lohmus (TU)

Organizing committee:
Prof. S. Tamulevičius (KTU) – *chairman*
Dr. R. Žostautienė (KTU) – *secretary*
Dr. E. Fataraitė-Urbonienė (KTU, ProTech)
Dr. A. Tamulevičienė (KTU)
Dr. T. Tamulevičius (KTU)
Dr. L. Puodžiukynas (KTU)
Dr. E. Rajackaitė (KTU)
PhD student T. Klinavičius (KTU)
PhD student M. Ilickas (KTU)
PhD student Š. Jankauskas (KTU)
V. Sinkevičienė (KTU)

Home page: http://advancedmaterials.ktu.edu/

Sponsors:

JSC “Inospectra”

JSC “Armgate”

JSC “Light Conversion”

JSC “Holtida”

JSC “Nanoversa”

“Optica” KTU Student Chapter

JSC “AkzoNobel Baltics”

“Beilstein Journal of Nanotechnology”

JSC “Mars Lietuva”

26th International Conference-School

ADVANCED MATERIALS AND TECHNOLOGIES

Programme

August 26, Monday

14:00 – 20:00 **Arrival and registration**

August 27, Tuesday

8:30 – 9:00 **Registration**

Chairperson Sigitas Tamulevičius

9:00 – 9:15 **Opening of the Conference-School**
Sigitas Tamulevičius (Kaunas University of Technology, Lithuania)

9:15 – 10:00 **Hubert Halbritter** (ams-OSRAM International GmbH, Germany)
Photons for a "Bright" Future

10:00 – 10:45 **Gintautas Tamulaitis** (Vilnius University, Lithuania)
Fast Scintillators for Fast Radiation Detectors in Demand for Future High Physics Experiments at CERN and High-Spatial-Resolution Medical Imaging Devices

10:45 – 11:05 Coffee Break

Chairperson Yogendra Kumar Mishra

11:05 – 11:50 **Evaldas Naujalis** (Centre for Physical Sciences and Technology, Lithuania)
Capabilities and Applications of Chromatography and Mass Spectrometry

11:50 – 12:20 **Evelina Dudutienė** (Centre for Physical Sciences and Technology, Lithuania)
Optical Characterization for Bismide-Based Quantum Structures Optimization

12:20 – 12:35 **Greta Bučytė** (JSC "Light Conversion", Lithuania)
Light Conversion for Ultrafast Spectroscopy

12:35 – 12:50 **Mindaugas Juodėnas** (Kaunas University of Technology, Lithuania)
RIANA: Research Infrastructure Access in Nanoscience & Nanotechnology

12:50 – 14:00 Break

14:00 – 16:00 **Social Event: 3x3 Basketball Tournament** (Palanga Vladas Jurgutis progymnasium, https://www.jurgucioprogimnazija.lt/, Ganyklų St. 2, Palanga)

16:00 – 18:00 Break

18:00 – 21:00 **Welcome Party** (Hotel Gabija Restaurant, Vytauto St. 40, Palanga)

August 28, Wednesday

8:30 – 9:00	**Registration**
	Chairperson Gintautas Tamulaitis
9:00 – 9:45	**Casper Kunstmann** (University of Southern Denmark, Denmark) **Gold Nanoparticle Based Thin Films for Optical and Electrical Sensing**
9:45 – 10:15	**Almira Ramanavičienė** (Vilnius University, Lithuania) **Recent Advances in Nanomaterial-Based Immunosensors**
10:15 – 11:00	**Yogendra Kumar Mishra** (University of Southern Denmark, Denmark) **Tetrapods based Smart Materials for Advanced Technologies**
11:00 – 11:20	Coffee Break
	Chairperson Igor A. Lukyanchuk
11:20 – 12:05	**Vaidas Klimkevičius** (Vilnius University, Lithuania) **Surface Modification of Nanoparticles: Challenges, Benefits and Applications**
12:05 – 12:35	**Weronika Andrzejewska** (Adam Mickiewicz University, Poland) **SARS-CoV-2 Nanobiosensor Based on Surface Plasmon Resonance**
12:35 – 13:20	**Vaidotas Marozas** (Kaunas University of Technology, Lithuania) **Photoplethysmography-Based Physiological Measurement Technologies: Applications and Uncertainty Estimation**
13:20 – 16:00	Break
16:00 – 21:00	**Social Event: Orienteering Competition, Exploring Lithuanian Kitchen** ("HBH Palanga", Žibininkai Village, http://www.hbh.lt/)

August 29, Thursday

8:30 – 9:00	**Registration**
	Chairperson Casper Kunstmann
9:00 – 9:45	**Igor A. Lukyanchuk** (Université de Picardie Jules Verne, France) **Fundamental Topology and Emergent Applications of the Nanostructured Ferroelectrics**
9:45 – 10:30	**Vyacheslavs Kashcheyevs** (University of Latvia, Latvia) **Recent Progress in Single-Electron Quantum Technologies**
10:30 – 11:15	**Andrei Kholkin** (University of Aveiro, Portugal) **Magnetoelectric Effect: Applications in Energy Harvesting and Biology**
11:15 – 11:35	Coffee Break
	Chairperson Vaidotas Marozas
11:35 – 12:20	**Dominik Farka** (Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Czech Republic) **Self-Assembly in the Service of Organic Electronics and Beyond**
12:20 – 13:05	**Kaspars Traskovskis** (Riga Technical University, Latvia) **Development of Light Emitting Two-Coordinate Copper(I) Complexes**
13:05 – 13:35	**Oleksandr Bezvikonnyi** (Kaunas University of Technology, Lithuania) **Exploitation of Triplet Emission in Organic Electroluminescent Devices and Optical Sensors**
13:35 – 15:30	Break
15:30 – 18:00	**Poster Session with Voting for the Best Poster** (*Chairperson Tomas Tamulevičius)*
18:00 – 18:30	**Best Poster Awards and Conference Photo**

August 30, Friday

Chairperson Kaspars Traskovskis

9:00 – 9:45	**Franz Faupel** (Kiel University, Germany) **Ways Out of the Climate and Sustainability Crisis - What Is Opinion, What Is Knowledge, Do We Have the Power to Change Something?**
9:45 – 10:30	**Denis Sokol** (Vilnius University, Lithuania) **Layered Double Hydroxide Structures (LDH): Fabrication Techniques and Diverse Applications**
10:30 – 10:40	Coffee Break

Chairperson Dominik Farka

10:40 – 11:10	**Krisjanis Smits** (University of Latvia, Latvia) **Advanced Characterization of Materials by SEM, TEM, FIB**
11:10 – 11:40	**Jurgis Pilipavičius** (Vilnius University, Lithuania) **Understanding of Materials Degradation in Aqueous Batteries**
11:40 – 11:50	**Closing Remarks**
11:50 – 12:30	**Certificates and Coffee Break**

LECTURES

Photons for a “Bright” Future

Hubert Halbritter, Martin Strassburg

ams-OSRAM International,
Leibnizstr. 4 93055 Regensburg, Germany
hubert.halbritter@ams-osram.com

Semiconductor based lighting components, in particular LEDs and LASER diodes have made enormous progress in the last decades. Early applications were simple indicator LEDs. In recent years LEDs enabled mobile devices, e.g. the illumination of displays or the flash of cameras. The recent improvements on the device level design and performance allows the rise of new applications beyond todays level.

The discussion covers the brief history of solid-state, semiconductor lighting components and their rapid development, their current status as well as an outlook into the future. In a second part, new technological developments and future potential applications and vice-versa are discussed. A particular focus is on system and component performance requirements based for future megatrends and applications beyond the state-of-the-art.

Fig. 1. Typ. Applications for LED and LASER based products

Keywords: *photonics, LED, Laser, optoelectronics.*

Fast Scintillators for Fast Radiation Detectors in Demand for Future High Physics Experiments at CERN and High-Spatial-Resolution Medical Imaging Device

Gintautas Tamulaitis

Institute of Photonics and Nanotechnology, Vilnius University
gintautas.tamulaitis@ff.vu.lt

A short introduction of CERN infrastructure, CERN future plans formulating the demands for the scintillation detectors of ionizing radiation with a special emphasis on the currently crucial demand for a substantially faster scintillation response that is also of especial importance in medical imaging, especially for positron emission tomography with time resolution, will be reviewed in this lecture. The lecture will show how the capabilities of the methods developed in materials science can be used for the development of fast scintillators, how optical techniques with time resolution might be employed for the characterization of fast scintillators, and how material engineering technics might be exploited for improving the timing properties of the future detectors of ionizing radiation.

Capabilities and Applications of Chromatography and Mass Spectrometry

Evaldas Naujalis[1,2]

[1]*State Research Institute Center for Physical Sciences and Technology, Savanorių Ave. 231, Vilnius, Lithuania*
evaldas.naujalis@ftmc.lt
[2]*Vilnius University Faculty of Chemistry and Geosciences Naugarduko St. 24, Vilnius, Lithuania*
evaldas.naujalis@chgf.vu.lt

Chromatography and mass spectrometry are ones of the most powerful analytical techniques widely used in various scientific fields for the separation, identification, and quantification of chemical compounds. Chromatography, including gas chromatography (GC) and liquid chromatography (LC), efficiently separates complex mixtures based on differential partitioning between a mobile phase and a stationary phase. Mass spectrometry (MS) provides detailed molecular information by measuring the mass-to-charge ratio of ionized compounds. The combination of chromatography and mass spectrometry (GC-MS and LC-MS) enhances analytical capabilities, offering high sensitivity, specificity, and the ability to analyze a wide range of substances. These techniques find applications in environmental analysis, pharmaceutical development, clinical diagnostics, food safety, forensic science, and among others.

In my presentation, I will explore the differences and recent developments in various chromatographic-mass spectrometric techniques. Additionally, I will showcase examples of their applications across different fields. Advances in these technologies continue to enhance their capabilities, establishing them as indispensable tools in modern analytical chemistry.

Keywords: *chromatography, mass spectrometry, analytical chemistry.*

Optical Characterization for Bismide-Based Quantum Structures Optimization

Evelina Dudutienė, Aistė Butkutė, Monika Jokubauskaitė, Bronislovas Čechavičius, Aivaras Špokas, Andrea Zelioli, Algirdas Jasinskas, Sandra Stanionytė, Martynas Skapas, Renata Butkutė

State Research Institute Center for Physical Sciences and Technology, Saulėtekio Ave. 3, LT-10257 Vilnius, Lithuania
evelina.dudutiene@ftmc.lt

One of the most intensively studied bismides is gallium arsenide bismide (GaAsBi). Rapid band gap energy (E_g) reduction up to 88 meV/%Bi, high spin-orbit splitting energy and lower E_g sensitivity to temperature make it promising material for active area of emitters operating in near-infrared spectral range. However, Bi incorporation within GaAs lattice is complicated and requires unconventional conditions of molecular beam epitaxy, such as low growth temperature (< 400ºC), near stoichiometric As/Ga ratio and etc. [1,2]. Also, since the atomic radius of the Bi atom is larger than those of Ga and As atoms, high Bi concentrations cause a lattice distortion. Therefore, emission efficiency of GaAsBi is low and optimization of growth and quantum structure design is essential for development of bismide-based optoelectronic devices. Photoluminescence (PL) spectroscopy is a powerful tool to study how technological approaches and structural design influence the optical properties of GaAsBi quantum structures. Moreover, PL is a non-destructive technique that requires no sample preparation, making it relatively simple and fast. Nevertheless, optical characterization allows for detailed investigation of observed physical processes, mechanisms, defects, etc.

In this talk several examples of how growth conditions, quantum structure design and post-growth treatment influence optical properties of GaAsBi quantum wells (QW) and how PL spectroscopy could be effectively used for quantum structure optimization. Temperature- and excitation-dependent PL results of two-substrate-temperature MBE growth approach, GaAsBi (QW) with linearly and parabolically graded AlGaAs barriers and post growth thermal annealing of GaAsBi QW with different barriers will be presented and discussed.

Acknowledgements: Part of this work was supported by Research Council of Lithuania under the Grant No. S-MIP-22-86.

Keywords: *GaAsBi, photoluminescence, MBE, NIR.*

References:

1. S. Francoeur et al. *Applied Physics Letters* **97(6)** p.11–14 (2006)
2. R. D. Richards et al. *Physica Status Solidi (b)* **259(2)** p. 2100330 (2022)

RIANA: Research Infrastructure Access in Nanoscience & Nanotechnology

Mindaugas Juodėnas[1], Sigitas Tamulevičius[1], Michael Stuckelberger[2]

[1]Institute of Materials Science, Kaunas University of Technology, K. Baršausko St. 59, LT-51423 Kaunas, Lithuania
[2]Deutsches Elektronen-Synchrotron DESY, X-Ray Nanoscience and X-Ray Optics, 22607 Hamburg, Germany
mindaugas.juodenas@ktu.lt

Research in nanoscience and nanotechnology is vital for global sustainability. Advancements in these fields rely heavily on research infrastructures (RIs). The EU-funded RIANA project [1] has brought together seven European networks of top-level RIs to provide access to the most advanced techniques for nanofabrication, processing/synthesis, characterization and analysis, as well as simulation capacity. Access to 69 infrastructures, spread across 22 European countries (fig.1), is efficiently coordinated through a single entry point. This access is facilitated by comprehensive scientific and innovation services offered by senior scientists, facility experts, and highly trained junior scientists.

The core objective of RIANA is to attract both experienced and new users from academia and industry. Priority will be given to researchers with the most innovative ideas and approaches that can effectively utilize the RIs for nanoscience and nanotechnology with a focus on sustainability. RIANA will accept user proposals based on a continuous call that will be launched soon. The excellence of user projects will be evaluated by an independent review panel using the following criteria: i) scientific excellence; ii) potential to increase technology readiness levels; iii) level of cross-disciplinarity; iv) impact on environmental safety; and v) impact on nanoscience or nanotechnology.

Fig. 1. The RIANA consortium encompasses 7 networks (LEAPS, Laserlab, e-DREAM, RADIATE, LENS, EuroNanoLab and EUSMI) offering access to 69 infrastructures, spread across 22 European countries

Keywords: *research infrastructures, sustainability, nanoscience, nanotechnology.*

References:

1. RIANA-project.eu

Funded by the European Union

Gold Nanoparticle Based Thin Films for Optical and Electrical Sensing

Casper Kunstmann[1], Mathias Brust[2]

[1]University of Southern Denmark, Mads Clausen Institute
Alsion 2, DK6400 Sønderborg, Denmark
[2]University of Liverpool, Department of Chemistry,
Crown Street, Liverpool L69 7ZD, United Kingdom
kunstmann@mci.sdu.dk

Thiolate-capped gold nanoparticles have been extensively studied over the past three decades. One of their most promising real life applications is the use of superlattices of particles as active components in artificial-nose-type sensing devices [1]. Here, we investigate the changes in interparticle spacing upon hydration and dehydration of drop-cast films of hydrophilic gold nanoparticles (GNP) have been measured in situ with nanometer resolution using WetSTEM and ESEM. These subtle variations correlate well with the corresponding changes in the optical spectra and perceived color as well as changes in the electrical conductivity of the films.

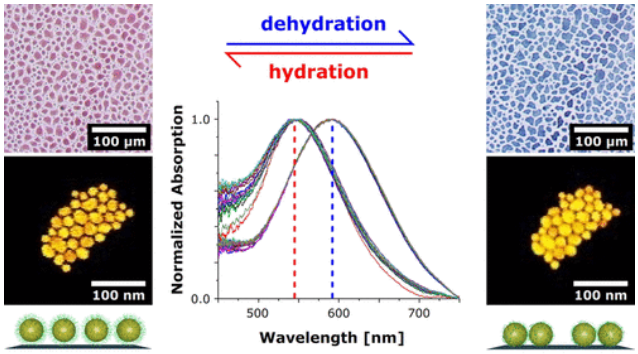

Fig. 1. Reversible humidity dependent optical spectra of GNP based thin films, observed under optical microscopy and high-resolution environmental SEM [2]

AC impedance analysis allows us to differentiate between resistive and capacitive components and to evaluate how these depend on average particle spacing and the water content of the matrix, respectively [2]. Thin films of this type are promising candidates for development of sensors and diagnostics.

Keywords: *nanoparticles, thin films, spectroscopy, environmental SEM, impedance.*

References:

1. H. Wohltjen et al. *Analytical Chemistry* **70** p. 2856−2859 (1998)
2. C. Kunstmann-Olsen et al. *Chemistry of Materials* **28(9)** p. 2970–2980 (2016)

Recent Advances in Nanomaterial-Based Immunosensors

Almira Ramanaviciene, Asta Kausaite-Minkstimiene, Benediktas Brasiunas, Anton Popov

NanoTechnas – Center of Nanotechnology and Materials Science, Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Naugarduko St. 24, LT-03225 Vilnius, Lithuania
almira.ramanaviciene@chf.vu.lt

Scientists are continuously investigating new technological approaches to develop sensitive, selective, rapid, cost-effective, and precise methods for the determination of biomarkers in body fluids. In this context, immunosensors are very promising and powerful diagnostic tools. The scientific and industrial impact of nanoscience and nanotechnology on the development of immunosensors has been growing fast. To construct ultra-sensitive immunosensors the advantages of different surface modification methods, various immunoassay formats, as well as innovative approaches based on the application of nanomaterials for the enhancement of the analytical signal need to be combined [1,2]. Noble metal and metal oxide nanoparticles have received considerable attention in the development of immunosensors due to their attractive physical and chemical properties and simple synthesis procedure.

In this contribution the trends and challenges in the applications of nanomaterials will be discussed, focusing particularly on the utilization of gold nanoparticles and magnetic nanoparticles modified by gold for the analytical signal amplification using direct and indirect biomarker detection strategies [3,4]. Additionally, the effects of nanoparticles on the optical and electrochemical immunosensor performance will be addressed.

Acknowledgments: This research was funded by a grant (No. S-MIP-22-46) from the Research Council of Lithuania.

Keywords: *electrochemical and optical immunosensors, gold nanoparticles, signal amplification strategies.*

References:

1. A. Ramanaviciene et al. In: The Detection of Biomarkers. Past, Present and the Future Prospects, 1st Edition, Eds: S. Ozkan, N. Bakirhan, F. Mollaraosouli. Elsevier, Academic Press (2022)
2. A. Popov et al. *Current Opinion in Electrochemistry* **46** p. 101524 (2024)
3. A. Kausaite-Minkstimiene et al. *ACS Appl. Mater. Interfaces* **14** p. 20720–20728 (2022)
4. B. Brasiunas et al. *Bioelectrochemistry* **156** p. 108638 (2024)

Tetrapods based Smart Materials for Advanced Technologies

Yogendra Kumar Mishra

Mads Clausen Institute, NanoSYD, Smart Materials,
University of Southern Denmark, Alsion 2, 6400 Sønderborg, Denmark
mishra@mci.sdu.dk

Considering the size dependent utilization complexities of nanoscopic dimensions towards real applications, the focus of nanomaterials community is merging to three-dimensional (3D) form of materials which are built out of interconnected anisotropic nanostructures. This talk will briefly introduce the importance of tetrapod shaped nanostructures towards smart 3D nanostructuring. A simple flame based single step approach was developed for synthesizing zinc oxide tetrapods which demonstrated many applications in different technologies. These tetrapods have been used as building blocks to construct highly porous interconnected 3D nanonetworks which can be utilized as templates to develop novel smart 3D networks from nearly any desired material. These smart 3D nanomaterials offer many applications in engineering and advanced technologies. Some examples of 3D nanomaterials engineering will be demonstrated along with their applications in various directions [1–10]. The scopes of 3D nanostructuring based smart materials in sensing, electronics, optoelectronics, energy, biomedical, optical and photonic engineering technologies, etc. will be briefly highlighted in the talk.

Keywords: *smart materials, tetrapods, hybrid nanomaterials, advanced technologies.*

References:
1. *Chemical Engineering Journal* **462** p. 141984 (2023)
2. *Progress in Materials Science* **139** p. 101169 (2023)
3. *Progress in Polymer Science* p. 101516 (2022)
4. *Materials Today* **50** p. 533–569 (2021)
5. *Materials Today* **48** p. 7–17 (2021)
6. *Advanced Science* p. 2100864 (2021)
7. *Advanced Functional Materials* **31** p. 20007555 (2021)
8. *Materials Today* **32** p. 108–130 (2020)
9. *Advanced Functional Materials* p. 1909725 (2020)
10. *Materials Today* **6** p. 631–651 (2018)

Surface Modification of Nanoparticles: Challenges, Benefits and Applications

Vaidas Klimkevičius

Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Naugarduko St. 24, LT-03225 Vilnius, Lithuania
vaidas.klimkevicius@chf.vu.lt

The rapidly expanding field of nanotechnology has seen remarkable progress with nanoparticles emerging as indispensable components across various sectors including healthcare, environmental remediation, electronics, energy, and materials science. Central to the utility of nanoparticles lies their surface modification, a process crucial for tailoring their properties to meet specific application requirements. This thesis explores the multifaceted landscape of nanoparticle surface modification, investigating the challenges, benefits, and diverse applications of this transformative technique.

Nanoparticles, owing to their small size and expansive surface area, harbor significant surface energy and often tend to agglomerate or aggregate. This underscores the critical importance of additional surface modification to ensure their stability in various media, including biological environments. Stability is a major issue hindering the widespread applicability of nanoparticles. However, it is not the only concern; some nanoparticles can be toxic to individuals or the environment. Therefore, surface modification is essential not only for stability but also to ensure the biocompatibility of these unique counterparts. Moreover, the targeted surface modification could tailor the surface properties empowering nanoparticles to overcome biological barriers, exhibit prolonged circulation times, and facilitate selective targeting in biomedical applications.

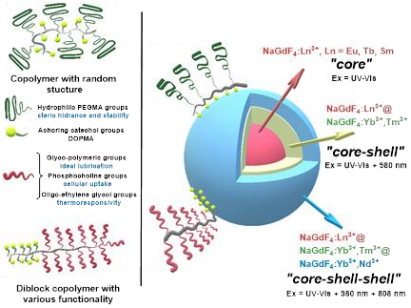

Fig. 1. Upconverting nanoparticles surface modification using various functional polymers

This presentation will focus on the development of multifunctional nanoplatforms for biomedical applications, encompassing synthesis methodologies, surface modification techniques and application capabilities.

Keywords: *optical nanoparticles, surface treatment, stability, biocompatibility, functionality.*

SARS-CoV-2 Nanobiosensor Based on Surface Plasmon Resonance

Weronika Andrzejewska[1], Nadzeya Khinevich[2], Patryk Obstarczyk[3], Szymon Murawka[1], Joanna Olesiak-Bańska[3], Sigitas Tamulevičius[2,4], Mikołaj Lewandowski[1]

[1]NanoBioMedical Centre, Adam Mickiewicz University, Wszechnicy Piastowskiej 3, 61-614 Poznań, Poland
[2]Institute of Materials Science of Kaunas University of Technology, K. Baršausko St. 59, LT-51423 Kaunas, Lithuania
[3]Institute of Advanced Materials, Wroclaw University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland
[4]Department of Physics, Kaunas University of Technology, Studentų St. 50, LT-51369 Kaunas, Lithuania
weronika.andrzejewska@amu.edu.pl

The COVID-19 pandemic has stimulated the scientific world to intensify studies aimed at developing quick and safe ways to detect viruses in human body. However, life-threatening virus studies can only be performed in certified laboratories that follow strict safety procedures. In other research units, the use of so-called virus-like particles (VLPs), in which the virus capsid is replaced by a synthetic core to which real virus proteins are attached [1], constitutes a safe alternative. The SARS-CoV-2 VLPs fabricated by our group are characterized by the presence of gold cores in which the so-called localized surface plasmon resonance (LSPR) appears [2]. Due to this, they can be applied in biosensing and bioimaging applications utilizing the surface-enhanced Raman scattering (SERS) [3]. In the next step, using the capillary-assisted particle assembly (CAPA) [4], we have prepared an innovative matrix composed of SARS-CoV-2 VLP exhibiting the surface lattice resonance. SERS signals originating from antibodies (mAbs) that specifically binding to VLPs make the fabricated system suitable for applications in ultrasensitive biodetection.

Acknowledgments: The studies were financed through the LaSensA project carried out under the M-ERA.NET scheme and co-funded by the European Union's Horizon 2020 programme, the Research Council of Lithuania (LMTLT), agreement No. S-M-ERA.NET-21-2, the Saxon State Ministry for Science, Culture and Tourism (Germany) and the National Science Centre of Poland, project No. 2020/02/Y/ST5/00086.

Keywords: *SARS-CoV-2, AuNPs, virus-like particles (VLPs), capillary-assisted particle assembly.*

References:

1. H. Tariq et al. *Frontiers in Microbiology* **12** p. 4137 (2022)
2. W. Andrzejewska et al. *ACS Synthetic Biology* **12(8)** p. 2320–2328 (2023)
3. N. Khinevich et al. *Sensors and Actuators B Chem*ical **394** p. 134418 (2023)
4. H. S. C. Yu. et al. *Particle & Particle Systems Characterization* **39(4)** p. 2100288 (2022)

Photoplethysmography-Based Physiological Measurement Technologies: Applications and Uncertainty Estimation

Vaidotas Marozas, Andrius Petrėnas, Andrius Sološenko, Mantas Rinkevičius, Arūnas Lukoševičius

Biomedical Engineering Institute, Kaunas University of Technology, K. Baršauskas St. 59, LT-51423 Kaunas, Lithuania
vaidotas.marozas@ktu.lt

Photoplethysmography (PPG) has emerged as a promising technology [1] in medical wearables for non-invasive monitoring of vital signs and pathologies such as heart arrhythmia [2] and blood pressure [3]. Although PPG-based devices offer convenience and accessibility, they also pose challenges related to uncertainty in measurement accuracy. This presentation explores the significance, sources, and methods for uncertainty estimation in PPG-based physiological measurements, critical for enhancing the trustworthiness of data obtained through medical wearables. Fig. 1 exemplifies two mentioned applications.

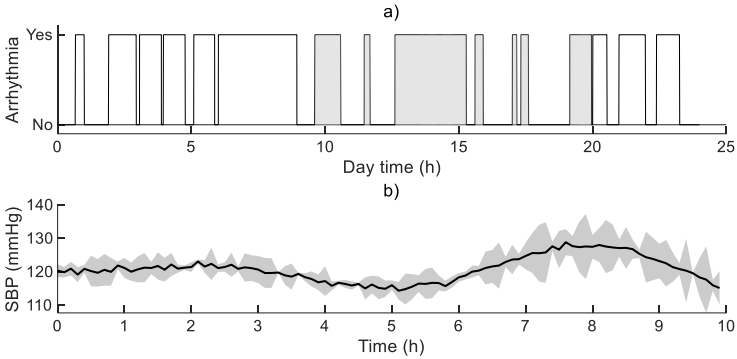

Fig. 1. PPG-based arrhythmia detection and systolic blood pressure (SBP) estimation. The shadowed area indicates uncertainty regions

Integration of uncertainty estimation methodologies, such as probabilistic, nonparametric modeling and error propagation analysis, into PPG-based systems, allows healthcare professionals better interpret and utilize the collected data for more confident clinical decision making.

Keywords: *PPG, medical wearable devices, heart arrhythmia, blood pressure, monitoring.*

References:

1. P. Charlton et al. *Physiological Measurement* **44** p. 111001 1–125 (2023)
2. A. Sološenko et al. *Physiological Measurement* **40(2)** p. 025003 1–13 (2019)
3. B. Paliakaitė et al. *Computing in Cardiology 2021* p. 1–4 (2021)

Fundamental Topology and Emergent Applications of the Nanostructured Ferroelectrics

Igor Lukyanchuk

University of Picardie, 33 rue St. Leu, 80000 Amiens, France
lukyanc@ferroix.net

The modern electronics is currently facing a profound challenge. The demand for even smaller and more closely packed elements has hit a stumbling block. We propose several solutions based on the unique functionality of electrically polarised nanomaterials, nanoferroelectrics, to host complex polarization textures that are incredibly stable due to topological self-protection

Negative capacitance [1] (NC) for low-dissipative nanoelectronics. We put forth a foundational mechanism of the NC demonstrating the inevitable emergence of the NC due to the formation of polarization domains. We establish a practical design of the NC FET based on the domain layout. The proposed device is tunable and downscales to the 2.5–5 nm technology node.

Ferroelectric THz vibrations [2] for ultrafast nanoelectronics. The suggested technology employs a ferroelectric material with a ferroelectric-dielectric heterostructure as a resonator for electrons of an electrical circuit or for a terahertz electromagnetic wave. A peculiarity of the described structure is that the polarization of each ferroelectric layer variates periodically in space, forming a set of domains that exhibits a diverse wealth of oscillation modes in the terahertz spectral band.

Ferroelectric tunable chirality [3] for optoelectronics. The topological chirality in nanostructured ferroelectrics is intimately related to topological polarization ordering. It emerges together with the polarization by spontaneous symmetry breaking from the non-chiral paraelectric state. In ferroelectrics it can be tuned and manipulated by changing the polarization ordering. Given that the latter is directly coupled to an electric field, the chirality switching, hence optical activity manipulation, by the electric field offers a remarkable operational platform.

Multilevel logic [4] unit for non von Neumann & neuromorphic computing. Ferroelectric nanodots hold two, three, or even four polarization states that are energetically stable thus providing a platform for encoding information. We reveal stable configurations and how to manipulate the polarization to move it between stable positions using electric fields. The important problems we address are the novel data protection and encryption protocols implementing these states and the ways the multilevel systems can enhance machine learning capable of better-emulating systems like the human brain.

Keywords: *ferroelectrics, topology, nanoelectronics.*

References:

1. I. Luk'yanchuk et al. *npj Computational Materials* **8(1)** p. 52 (2022)
2. I. Lukyanchuk *VM Vinokur Physical Review B* **98** p. 024107 (2018)
3. I. Luk'yanchuk et al. arXiv preprint arXiv:2406.19728 (2024)
4. L. Baudry et al. *VM Vinokur Scientific reports* **7(1)** p. 42196 (2017)

Recent Progress in Single-Electron Quantum Technologies

Vyacheslavs Kashcheyevs

Department of Physics, Faculty of Exact Sciences and Technologies,
University of Latvia, Jelgavas St. 3, LV-1004 Riga, Latvia
vjaceslavs.kascejevs@lu.lv

Universality of electrical charge quantization and the fundamental nature of the Planck constant are the foundational principles of electrical quantum metrology where macroscopic quantum phenomena (quantum Hall and Josephson effects) are routinely employed in commercial high-precision measurements systems. Recent advances in high-fidelity manipulation of discrete electrons in metrological current sources [1] open up a new resource for quantum technologies 2.0 [2] with individual electrons propagating in semiconductor circuits in direct analogy to photons. We discuss an electron quantum optics toolbox of circuit elements for on-demand emission, transformation, and read-out of single-electron wave-packets, emphasizing the unique advantages of beamsplitters [3,4] with the dispersion tuneable by the field effect and the non-linearity mediated by controlled Coulomb interaction. Envisioned applications are quantum-limited sensors for picosecond scale electrical signals and eventually an all-electronic quantum information platform interfaceable with other cryogenic on-chip technologies.

Keywords: *quantum technologies, single-electron devices, metrology, quantum optics.*

References:

1. B. Kaestner, V. Kashcheyevs *Reports on Progress in Physics* **78** p. 103901 (2015)
2. S. Cinà et al. Strategic Research and Industry Agenda 2030: Roadmap and Quantum Ambitions over this Decade, qt.eu/publications (2024)
3. J. Fletcher et al. *Nature Communications* **10** p. 5298 (2019)
4. N. Ubbelohde et al. *Nature Nanotechnology* **18** p. 733 (2023)

Magnetoelectric Effect: Applications in Energy Harvesting and Biology

Andrei Kholkin

Department of Physics & CICECO – Aveiro Institute of Materials, University of Aveiro, Campus Universitario de Santiago, 3810–193 Aveiro, Portugal
kholkin@ua.pt

Magnetoelectric (ME) effect is defined as a linear coupling between polarization and magnetic field (direct effect) and between magnetization and electric field (converse effect). This effect has been of immense interest in the scientific community over the past years [1]. Unlike ME of single-phase multiferroics, numerous ME composites, combining elastically coupled piezoelectric and magnetostrictive phases, have been shown to yield very strong ME effects even at room temperature. These structures also offer a great flexibility in the sense that a large number of parameters may be tuned independently including the materials properties of the constituent phases and the connectivity between them. Consequently, these composites are nowadays very close to a range of promising applications including: DC and AC magnetic vector field and electric current sensors, magneto-electro-elastic energy harvesters, multiple-state memory devices, micro-sensors in read heads, transformers, spinners, diodes, spin-wave generators, electrically tunable microwave filters, and various biomedical devices.

In this work, the fabrication and characterization of several types of novel ME composite transducers will be presented including magnetic/piezoelectric cantilevers for environmental (mechanical+magnetic) energy harvesting [2], sensitive magnetic field sensors, and various ME composites (scaffolds) for tissue regeneration, drug delivery, and remotely induced catalysis. These include piezoelectric fibers with embedded magnetic nanoparticles, ME nanorods, and core-shell ME spherical nanoparticles. These composites are characterized by excellent biocompatibility and biodegradability and show large ME response mediated by the remote magnetic field. Scaffold morphology, molecular and phase composition, crystalline structure, surface potential, and local piezoresponse were studied [3]. Core-shell structures based on $MnFe_2O_4$ and $(Ba,Ca)(Zr,Ti)O_3$ were synthesized by mild hydrothermal synthesis and surface modification [4]. These structures were used for the removal of water pollutant (rhodamine B) with more than 95% efficiency under AC magnetic field of only 150 mT. Other examples of the biomedical applications of ME composites will be presented in this talk.

Keywords: *magnetoelectric effect, energy harvesting, magnetic field sensors, tissue.*

References:

1. S. Kopyl et al. *Materials Today Bio* **12** p. 100149 (2021)
2. J. V. Vidal et al. *IEEE Trans. Ultrason. Ferroelectr. & Freq. Control* **67** p. 1219 (2020)
3. R. V. Chernozem et al. *Nano Energy* **89** p. 106473 (2021)
4. R. V. Chernozem et al. *Small* p. 2302808 (2023)

Self-Assembly in Conductive Polymers: Towards Improved Organic Electronics and Beyond

Dominik Farka

Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Flemingovo Náměstí 2, 160 00 Prague, Czech Republic
dominik.farka@uochb.cas.cz

The role of organic conductors, in particular the role of conductive polymers has steadily increased over the past years as robust, highly-conductive polymers emerged. Therein, their efficient charge-transport presents a pressing issue in the field organic electronics. Poly(3,4-ethylenedioxythiophene) (PEDOT) has emerged as the dominant material in the field and most optimization and applications have focussed in this material [1].

In this talk, we will focus on alternatives to processing optimization, specifically on oxidative chemical vapour deposition (oCVD) of PEDOT [2,3] and other, emerging materials. Through the employment of functional doping agents and functionalization of surfaces by self-assembled monolayers (SAMs), high conductivities are possible even in materials notorious for limited conductivities.

The results will be supported with XPS, XRD, GIWAXS, AFM/KFM measurements and theoretical studies that aim to explain the mechanisms involved.

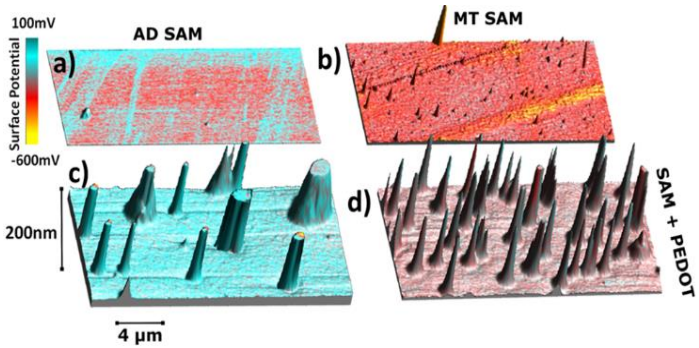

Fig. 1. Tremendous effect of a self-assembled monolayer (SAM) on topography and surface potential (~work function) of deposited PEDOT [4]

References:

1. M. N. Gueye et al. *Progress in Materials Science* **108** p. 100616 (2020)
2. M. Heydari Gharahcheshmeh et al. *Adv. Funct. Mater.* **31(14)** p. 2008712 (2021)
3. D. Farka et al. *AEM* **3(7)** p. 1700050 (2017)
4. D. H. Apaydin et al. *ACS Appl. Nano Mater.* **5(3)** (2022)

Development of Light Emitting Two-Coordinate Copper(I) Complexes

Kaspars Traskovskis, Armands Ruduss

Faculty of Natural Sciences and Technology, Institute of Chemistry and Chemical Technology, Riga Technical University, Paula Valdena St. 3, LV-1048 Riga, Latvia
kaspars.traskovskis@rtu.lv

In recent years the focal point of organic light emitting diode (OLED) emitter development has shifted towards the search for cheaper and more sustainable alternatives for the widely used heavy transition metal complexes (such as Ir, Pt). One of the explored directions involves the acquisition of two-coordinate coinage metal (Cu, Ag, Au) complexes bearing electron deficient carbene and electron rich amide ligands (fig. 1). These compounds exhibit highly efficient thermally activated delayed fluorescence (TADF) characterized with low photoluminescence lifetimes (below 1 μs) and near-unity photoluminescence quantum yields, making them suitable for OLED applications [1].

Recently we have discovered yet unknown photophysical characteristics of this compound class that open novel practical application directions. Firstly, by using specific carbene ligands with axillary acceptor fragments we were able to induce through-space interligand charge transfer process, associated with TADF with very low activation energy [2].

We have also shown that by incorporating carbene ligands with reduced sterical shielding the formation of emissive dimers can be achieved for the corresponding complexes. In this case the emissive charge transfer process proceeds between face-to-face aligned donor and acceptor fragments of the neighboring molecules. The dual emission form monomeric and dimeric complex species results in white emission that can be exploited to produce cost-effective simple design white light OLEDs [3,4].

Finally, by choosing donor fragments with energetically low-laying local triplet states, long-lived room temperature phosphorescence can be induced in the materials that can be used for oxygen sensing or for production of anti-counterfeit markers.

Keywords: *TADF, OLED, copper complex, phosphorescence.*

References:

1. T.-Y. Li et al. *Chemical Reviews* **124(7)** p. 4332–4392 (2024)
2. A. Ruduss et al. *Inorganic Chemistry* **61(4)** p. 2174–2185 (2022)
3. A. Ruduss et al. *ACS Applied Materials & Interfaces* **14(13)** p. 15478–15493 (2022)
4. A. Ruduss et al. *Physical Chemistry Chemical Physics* **25** p. 3220–3231 (2023)

Exploitation of Triplet Emission in Organic Electroluminescent Devices and Optical Sensors

Oleksandr Bezvikonnyi[1,2]

[1]*Department of Polymer Chemistry and Technology, Kaunas University of Technology, K. Baršausko St. 59, LT-51423 Kaunas, Lithuania*
[2]*Department of Physics, Kaunas University of Technology, Studentų St. 50, LT-51368 Kaunas, Lithuania*
o.bezvikonnyi@ktu.lt

Organic light emitting diodes (OLED) have undergone rapid development recently in the market of displays and lighting devices. Nevertheless, the biggest challenge for the technology remains the demand for higher efficiency, especially for blue emitting devices. As the singlet and triplet excitons are formed in a ratio 1 to 3 in OLEDs, the logical way to increase the efficiency of device is the exploitation of the triplet excited states.

The phosphorescent emitters possess metal atoms incorporated in the organic complexes. This helps to enhance spin-orbit coupling making spin-forbidden transitions emissive at room temperature. The incorporation of heavy atoms such as sulphur was suggested as the way to achieve room temperature phosphorescence (RTP) of fully organic emitters without noble metals such as Ir, Pt, etc. [1]. The alternative to the phosphorescent OLEDs is the devices based on the phenomenon of thermally activated delayed fluorescence (TADF). TADF is the delayed fluorescence of upconverted triplet excitons through the reverse intersystem crossing [2]. TADF requires the charge transfer for the minimization of singlet-triplet energy splitting. Thus, the donor-acceptor moieties are required within a molecule or exciplex-forming molecular mixtures. If the charge transfer is localized, the multiresonant TADF occurs. It results in the significant reduction of full width at half maximum of emission and enhancement of stability and efficiency of OLEDs [2]. The collisional interactions with molecular oxygen quench triplet emission. In the case of RTP, an additional spectral band appears after the removal of oxygen, unlike in case of TADF. Such unique dependence on oxygen makes it possible to utilize TADF and phosphorescent emitters for optical sensors of oxygen. Hyperfluorescence was introduced to narrow the emission spectral band, and to improve device stability and efficiency [2]. It is based on the utilization of host-sensitizer-guest systems in which triplet harvesting happens in the host compounds and then the conventional prompt fluorescent emitter can emit light with increased efficiency. The combination of TADF, RTP, solid state luminescence enhancement and mechanochromism is considered recently.

In this presentation our work related to the study and exploitation in OLEDs and optical sensors of the emissions facilitated by triplet excitons will be reviewed.

Keywords: *triplet, OLED, sensor, TADF, RTP, hyperfluorescence.*

References:

1. Y. Patil et al. *Chirality* **35(7)** p. 390–410 (2023)
2. E. Tankelevičiūte et al. *The Journal of Physical Chemistry Letters* **15** p. 1034–1047 (2024)

Ways out of the Climate and Sustainability Crisis – What is Opinion, What is Knowledge, do We Have the Power to Change Something?

Franz Faupel

Chair for Multicomponent Materials, Department of Materials Science, Kiel University, Kaiserstraße 2, 24143 Kiel, Germany
ff@tf.uni-kiel.de

The climate and sustainability crisis is currently the biggest problem for the survival of humanity. It cannot be solved by science and technological progress alone but requires a change of thinking at all levels. As scientists, we have a special responsibility and should take a leading role in communicating the need for urgent action to the public and decision makers.

The first part of this talk will highlight the alarming signals, which are meanwhile also clearly visible in Europe. Our climate exhibits the typical features of a strongly interconnected complex system, such as strong nonlinearities, positive feedback, and tipping points, which are characterized by massive irreversible changes and cascade effects. Due to the well-known exponential growth effects in complex systems, there is not much time left before the first tipping points are reached.

The second part of the talk addresses the question of what are the barriers towards change despite the striking evidence and what can be done. Based on examples from Kiel and our very active network *North European Network Nanotechnology* (NINa e.V., https://www.nina-sh.de) it will be shown that nanotechnology and new materials are key technologies to overcome the climate crisis. Emphasis, however, will be put on a more general view, ranging from the role of universities and the scientific community to our lifestyle. A sustainable lifestyle and a focus on what is important in life would not only improve our quality of life but also solve many other problems. This has particularly been demonstrated over the last years by Finland, which is the leading nation in terms of sustainability [1] and continues to have the happiest people worldwide [2].

As for the scientific community, we, a group of concerned researchers, recently founded the *International Alliance of Societies for a Sustainable Future* (https://sfs-alliance.org). Our vision is to establish an international scientific network as a tool to alert the general public worldwide to the sustainability crisis and to recommend measures for a socio-ecological transformation [3]. The alliance is not restricted to natural sciences and technology but aims to go through all disciplines across borders and cultures.

Keywords: *sustainability, climate crisis, alliance of scientific societies.*

References:

1. J. F. Helliwell et al. (Eds.). World Happiness Report 2023 (11th ed.). Sustainable Development Solutions Network (2023)
2. J. D. Sach et al. Sustainable Development Report 2023. Paris: SDSN, Dublin: Dublin University Press (2023)
3. J. Rödel et al. *J. Mater Sci.* **58** p. 15577–15587 (2023)

Layered Double Hydroxide Structures (LDH): Fabrication Techniques and Diverse Applications

Denis Sokol, Neringa Gailiūtė, Aivaras Kareiva

Faculty of Chemistry and Geociences, Institute of Chemistry, Vilnius University, Naugarduko St. 24, LT-03225 Vilnius, Lithuania
denis.sokol@chgf.vu.lt

In recent years, layered double hydroxides (LDHs) have attracted great attention from scientists due to their wide and important spectrum of applications in different areas such as catalysis, photochemistry, biomedical science, and the environment [1]. Nowadays, the most common synthesis techniques for LDH fabrication are co-precipitation or hydrothermal methods, but other methods like sol-gel, anion exchange, or ball milling are also used. Each of these above-mentioned methods has its own advantages and disadvantages when compared to each other, especially for some specific applications [2].

The aim of this study is to show how the dual-stage co-precipitation method can be used to synthesize different metal composition LDHs inside the wood matrix. Mineralization of wood blocks occurs in multiple steps: vacuuming, soaking with different compositions and concentrations of M2+/M3+ metal nitrate solutions, drying of wood, and again repeating the same procedure but with a second soaking in sodium carbonate (Na_2CO_3) solution (see fig. 1). The properties of mineralized wood samples, such as mechanical strength, thermal insulation, fire retardancy, antibacterial, and antifungal properties, have been investigated and show a high potential for application.

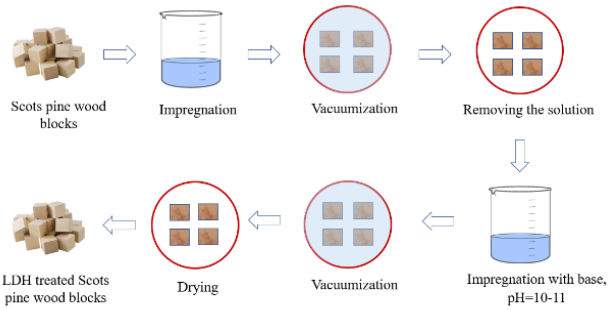

Fig. 1. Schematic diagram of wood impregnation

Keywords: *sol-gel, co-precipitation, layered double hydroxide, wood mineralisation, soaking.*

References:

1. U. A. Mohanty et al. *Sustain. Energy Fuels* ***7*** p. 1145–1186 (2023)
2. F. L. Theiss et al. *Appl. Surf. Sci.* ***383*** p. 200–213 (2016)

Advanced Characterization of Materials by SEM, TEM, FIB

Krisjanis Smits[1,2]

[1]*Institute of Solid State Physics, University of Latvia, Kengaraga St. 8, LV1063 Riga, Latvia*
[2]*Institute of Biomaterials and Bioengineering, Riga Technical University, Paula Valdena St. 3, 1048, Riga, Latvia*
smits@cfi.lu.lv

With the reduction of device sizes and materials to nanoscale dimensions, electron microscopy has emerged as a widely used method for characterizing materials in the field of material science. Throughout the last century, electron microscopy techniques have experienced consistent advancements and innovation. This presentation will focus on conventional electron microscopy techniques and discuss my experience in materials science with these powerful instruments.

The primary emphasis will be on advanced measurement techniques, namely scanning electron microscopy (SEM), focused ion beam (FIB), and transmission electron microscopy (TEM), with a particular focus on the SEM FIB Helios 5UX system. These integrated systems merge scanning electron microscopy (SEM), focused ion beam (FIB), and transmission electron microscopy (TEM) to offer a thorough analysis of samples. This includes examining the surface, analysing the elements present, obtaining topographical information, and creating three-dimensional reconstructions. Scanning Electron Microscopy (SEM) provides detailed images of surfaces, allowing for analysis of the elements present and crystal structure. The Focused Ion Beam (FIB) prepares lamellae by slicing and viewing study materials in bulk, removing them, and creating patterns on them. Transmission electron microscopy (TEM) allows for extremely detailed imaging at the atomic level and provides crystallographic data. Furthermore, modern electron microscopy systems enable various analytical techniques, in situ measurements, and prototyping, thereby greatly expanding their analytical capabilities.

The presentation will provide an introduction to the fundamental principles of electron microscopy, highlight practical applications in the field of material science, and delve into the most recent advancements in these technologies. These advancements create opportunities to analyse intricate materials, nanostructures, and biomaterials, fostering innovation in diverse fields such as material science, electronics, and biotechnology. The purpose of this lecture is to offer knowledge and understanding of the practical uses and potential future advancements of these highly effective tools in the field of material science.

Keywords: *SEM, FIB, TEM.*

Understanding of Materials Degradation in Aqueous Batteries

Jurgis Pilipavicius[1,2], Nadezda Traskina[1], Gintare Gece[1], Jurga Juodkazyte[1], Linas Vilciauskas[1,2]

[1]Department of Chemical Engineering and Technology, Center for Physical Sciences and Technology
[2]Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University
jurgis.pilipavicius@chf.vu.lt

Novel technological solutions are required for the rapid transition to renewable energy and sustainable material ecosystems. There is widespread agreement that various electrochemical technologies for energy and catalytic conversion, material processing, and recycling will be key to this transition [1,2]. The main advantages of electrochemical devices are their high efficiency and process selectivity, as well as their unique scalability [3]. Aqueous batteries based on Na or Zn ions are gaining attention for stationary energy storage because of their cost-effectiveness, safety, and environmental benefits, where low specific capacity is not a major concern. Na superconductors (NASICONs) and Prussian blue analogs (PBAs) are good candidates as potential electrode materials for this type of battery technology. Both have a rigid three-dimensional structure that allows easy insertion or extraction of ions. However, in aqueous media, these materials often suffer from low coulombic efficiency, fast self-discharge, and rapid capacity fade. These effects are still poorly understood, and a better understanding of their origin is crucial for their mitigation.

In this study, we investigated a range of NASICONs, including $NaTi_2(PO_4)_3$, $NaTiMn(PO_4)_3$, $Na_2TiV(PO_4)_3$, and PBA materials, such as $Na_2Fe_2(CN)_6$-xH_2O. To understand the underlying degradation mechanisms of these materials, we studied their electrochemical performance in aqueous systems using a combination of electrochemical and other techniques such as operando pH measurements, ex situ X-ray diffraction and Rietveld refinement, solid-state NMR, and XPS. We demonstrated that the control of dissolved oxygen, pH, and battery operating conditions plays a major role in the degradation of these materials. Based on the collected data, we developed several strategies to mitigate these effects, such as ALD coatings, tuning of the electrolyte composition, and utilization of reducing agents.

Keywords: *NASICON, PBA, aqueous battery.*

References:

1. V. R. Stamenkovic et al. *Nature Materials* **16** p. 57–69 (2016)
2. S. Möhle et al. *Angewandte Chemie International Edition* **57** p. 6018–6041 (2018)
3. M. A. Alkhadra et al. *Chemical Reviews* **122** p. 13547–13635 (2022)

POSTER PRESENTATIONS

METHODS OF SURFACE ANALYSIS

P1-P7

P1. Leidenfrost Temperature of Aluminium Samples and Vapour Layer Formation under Boiling Crisis Condition

Ala Gassim Elhag Elshakh Mohamed, Raminta Skvorčinskienė

Lithuanian Energy Institute, Breslaujos St. 3, LT-44403 Kaunas, Lithuania
ala.gasim@lei.It

Leidenfrost regime occurs when a liquid brought into contact with superheated solid surface, the effect has been discovered earlier by the scientist Johann Gottlob Leidenfrost in 1856. When the temperature increases and also the heat flux increases to be closer to the critical heat flux, then they will be a vapour layer to insulate the surface, hence, prevent the heat transfer and leads to a frictionless state, the determination of Leidenfrost temperature is crucial in numerous applications, including but not limited to fuel injection, spray cooling, and drag reduction [1,2]. In this work, Leidenfrost temperature for aluminum samples were determined for different sample's temperature, water temperature. Aluminum samples are heated up to, 300, 320, and 340°C, also the T_{water} was changed at each time (20, 25, 30°C). The setup of Leidenfrost experiment as in fig 1.

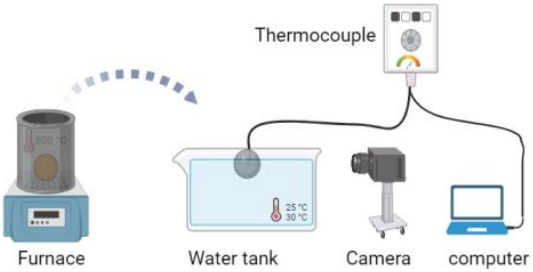

Fig. 1. Represents Leidenfrost effect setup

The results were shown that the formation of the vapor film and Leidenfrost effect, further studies will be done to lower Leidenfrost temperature by texturing and coating the aluminium samples.

Keywords: *boiling crisis, vapour film, critical heat flux, and Leidenfrost temperature.*

References:

1. J. Gylys et al. *International Journal of Heat and Mass Transfer* **89** p. 913–919 (2015)
2. Q. Zhang et al. *Applied Surface Science* **280** p. 545–549 (2013)

P2. Is the Biogas Production Waste a Suitable Source of Plants Nutrients?

Eglė Didžiulytė, Rasa Šlinkšienė

Department of Physical and Inorganic Chemistry, Kaunas University of Technology, Radvilėnų Rd. 19, LT-50254 Kaunas, Lithuania
egle.didziulyte@ktu.lt

The main purpose of agriculture is food supply, and the application of effective methods allows to grow large quantities of quality crops. However, extremely intensive and chemicalized agriculture severely damages the naturally formed ecosystem [1]. It is this problem that encourages concern about soil conservation, improving its quality, human health, and environmental protection, which encourages the search for alternative methods of agriculture. One of them is organic farming, which is a method in which mineral fertilizers are not used, and nutrients needed by plants are provided using biological substances of organic origin. One of them is biogas production waste – digestate, which regulates soil structure because it is rich in organic matter. Scientific studies confirm that biogas digestate is used as fertilizers for plants, as a soil improver, as a biological product in the fight against diseases and pests, and as a substrate in hydroponics [2].

A chemical analysis of the three companies digestate samples was carried out, which showed that the digestates contain primary and secondary nutrients. In order to produce high-quality fertilizers or a base for growing plants, it is very important to know not only the chemical composition, but also the structure of the materials, their homogeneity and surface. Therefore, the digestate was analysed by the SEM-EDS method, taking photos of the raw materials, elemental mapping, and the concentration of elements (fig.1).

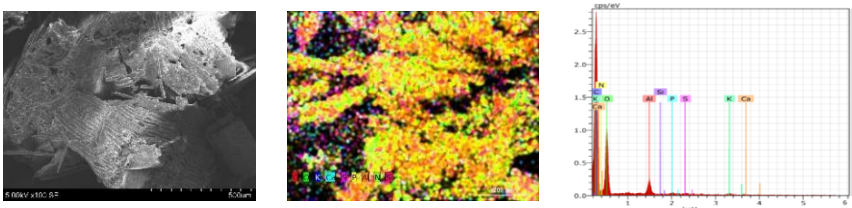

Fig. 1. SEM-EDS photo and elemental mapping of raw material (*Kurana*, Pasvalys)

Keywords: *digestate, organic farming, fertilizers, element map.*

References:

1. S. J. Parikh et al. *Nature Education Knowledge* **3(10)**:2 (2012)
2. J. Paull *European Journal of Social Sciences* **21(1)** p. 64–70 (2011)

P3. Atomic Force Microscopy Characterization of Human Lung Cancer Tissue

Lāsma Bugovecka[1], Uldis Maļinovskis[1], Sergejs Isajevs[2], Andis Liepiņš[3], Donāts Erts[1]

[1]Institute of Chemical Physics, University of Latvia, Jelgavas Street 1, LV-1004 Riga, Latvia
[2]University of Latvia, Faculty of Medicine, Department of Pathology, Jelgavas Street 3, LV-1004 Riga, Latvia
[3]LLC „ APPLY", Ieriķu Street 5, LV-1084 Riga, Latvia
lasma.bugovecka@lu.lv

The study of human lung cancer is crucial due to its status as a leading cause of cancer-related deaths worldwide. Different subtypes of lung cancer exhibit unique characteristics, making it important to understand their morphological and molecular features. Atomic Force Microscopy (AFM) is a powerful tool for studying lung cancer tissues, offering high-resolution imaging at the nanoscale, and measuring tissue mechanical properties such as stiffness and elasticity, which are indicative of cancer progression [1]. While AFM has been used to study various cancers, its application to human lung cancer tissues remains largely unexplored. This presents an opportunity to discover novel properties of lung cancer subtypes.

In this study, we investigated the potential of AFM methods in analysing human lung cancer tissue using histologically relevant biopsy preparation techniques. Adenocarcinoma and squamous cell carcinoma tissue samples were prepared using cryosectioning to obtain tissue slices and using liquid-based cytology for single cell samples. Tissue sections ranging from 5–10 µm thickness and scan areas from 2x2 to 60x60 µm^2 were examined using AFM tapping mode, achieving good image quality, and finding many micro-structured regions (see fig. 1). Cytological samples were prepared for cell surface morphology and viscoelasticity studies, measured in contact mode, successfully obtaining single cell images (see fig. 1). Additionally, different cell chemical fixation methods were compared using cell cultures to optimize AFM techniques.

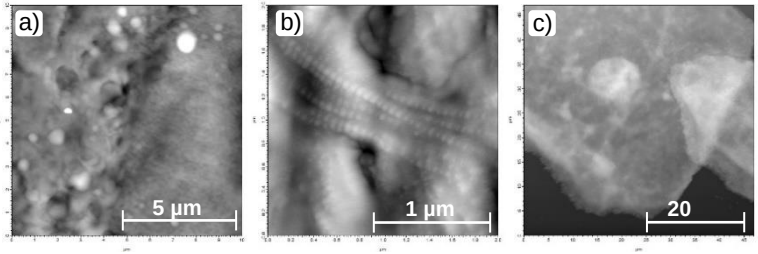

Fig. 1. AFM a) amplitude image of a 10x10 µm^2 area and b) height image of 2x2 µm^2 area of human lung cancer tissue sections, and c) 47x47 µm^2 area of a cytological sample

Keywords: *atomic force microscopy, human lung cancer, tissue sections.*

References:

1. J. Malhotra et al. *European Respiratory Journal* **48** p. 889–902 (2016)

P4. Investigation of Nanobodies and SARS-CoV-2 S Protein Interaction in Real-time by Complementary Surface Sensitive Optical and Acoustic Methods

Miglė Stančiauskaitė[1], Silvija Juciutė[1], Vincentas Mačiulis[2], Ieva Plikusienė[1]

[1]NanoTechnas – Center of Nanotechnology and Materials Science, Faculty of Chemistry and Geosciences, Vilnius University, Vilnius, Lithuania
[2]State Research Institute Center for Physical Sciences and Technology, Vilnius, Lithuania

The pharmaceutical industry has increasingly used antibodies (ABs), which are effective but limited by their instability and high molecular weight (~150 kDa), reducing tissue penetration. Nanobodies (NBs) are antigen-binding proteins derived from ABs found in Camelidae, composed only of a heavy chain with a variable domain that has antigen-binding capability. Their shape allows access to binding sites that may be unreachable for conventional ABs. NBs investigated as agents for immunotherapy can also be employed in biosensing. Using NBs in Surface Plasmon Resonance imaging offers increased sensitivity due to higher ligand density and more detectable space [1].

To prevent random AB orientation, site-oriented AB immobilization through protein G can be used to enhance AB density and increase antigen binding activity. This type of sandwich assay allows AB regeneration, allowing multiple measurements during the same experiment. The main target in combating SARS-CoV-2 is the S protein, which is responsible for binding to the ACE2 receptors of host cells [2]. NBs have been engineered to bind to both active and inactive conformations of the receptor-binding motif (RBM) of the receptor-binding domain (RBD) of the S protein, thus preventing viral entry into the cell.

In the present work we applied label-free, real-time, non-destructive surface sensitive methods of spectroscopic ellipsometry and quartz crystal microbalance to investigate real-time interaction of NBs specific to SARS-CoV-2 S protein. Simultaneous QCM and ellipsometry measurements allow to precisely calculate antigen binding affinity and surface mass density, resulting in a deeper understanding of different SARS-CoV-2 variant detection.

References:

1. R. Chen et al. *Sens Actuators B Chem* **395** p. 134490 (2023)
2. W. Wang et al. *Biochem Pharmacol* **208** p. 115401 (2023)

P5. High Energy Electron Radiation Dose Influence on Exoelectron Emission of Monocrystalline Silicon

Gaļina Boka[1], Yuri Dekhtyar[2], Mirko Rocca[2], Elizabete Skrebele[2]

[1]Riga Technical university, Ķīpsalas Street 6B, LV-1048 Riga, Latvia
[2]Oncology Centre of Latvia, Hipokrāta Street 4, LV-1038 Riga, Latvia
Elizabete.Skrebele@edu.rtu.lv

High energy electron radiation (4 to 22 MeV), used for radiotherapy [1], induces the formation of the complex point defects in the monocrystalline Si [2]. If irradiated Si is simultaneously heated and exposed to ultraviolet radiation (UV) (photon energy is close to work function of Si) exoelectron emission (EEE) appears [2]. While Si EEE can be used for detection of absorbed dose delivered by5 MeV electrons, its dependence on energies >5 MeV stays unrevealed.

Crystalline p-type Si (10 Ω*cm) was irradiated with 6 MeV electron beam, typical for radiotherapy, with LINAC Varian TrueBeam. Irradiated Si specimens were measured to meet EEE (heat pace 10°C/min, UV photon energy 4.4 eV).

The EEE emission current I_e has a peak at 500–550°C (fig.1) connected with Si-H/ Si-O bonds reconstruction [4]. An increment of derivation (dI_e/dT) of the EEE peak correlates with the delivered dose (fig. 2).

The result indicates potential of EEE for detection of the dose (12–60 Gy) delivered with 6 MeV electron beam.

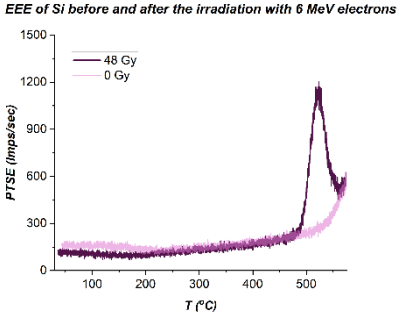

Fig. 1. Exoelectron emission of Si before and after irradiation with 6 MeV electrons

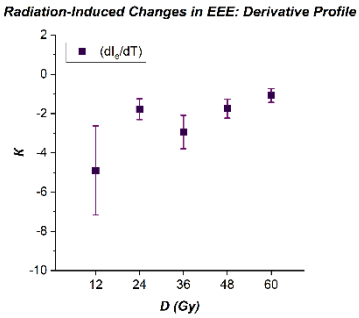

Fig. 2. 6 MeV electron dose influence on exoelectron emission of Si

Keywords: *exoelectron emission, monocrystalline silicon, electron beam radiation, dosimetry.*

References:

1. E. B. Podgorsak (editor) *Radiation oncology physics: a handbook for teachers and students* p. 273–299 (2005)
2. Yu. Dekhtyar et al. *Journal of Applied Physics* **75(8)** p. 4201–4207 (1994)
3. Yu. Dekhtyar et al. *Phys. Stat. Sol.* **102(2)** p. 665–677 (1987)
4. J. Jeurink et al. *Proc. 26th EU PVSEC* (2011)

P6. Study of the Properties of Resistance Welded Joints of Microcomposite Conductors

Paulius Beinoras, Nikolaj Višniakov, Oleksandr Kapustynskyi

VilniusTECH – Vilnius Gediminas Technical University, Saulėtekio Ave. 11, LT-10223 Vilnius, Lithuania
paulius.beinoras@vilniustech.lt

In modern fundamental and applied research, as well as in the most innovative industrial processes, systems with strong magnetic fields are widely used [1]. These devices generate magnetic fields with strengths ranging from 5 to 100 T, and the conductors experience immense Lorentz forces [2]. Therefore, the material of the conductors must be extremely strong (tensile strength not less than 700 MPa) and have good specific electrical conductivity (IACS ≥ 60%).

Traditional conductors such as copper, aluminum, gold, and silver cannot withstand these loads. Consequently, microcomposite materials have been developed, which exhibit high strength and good specific electrical conductivity. One of the significant unresolved problems in systems with strong magnetic fields is the creation of reliable non-destructive joints and the search for reliable joining technologies, as most such magnet structures must remain intact once they are in operation. However, the commonly used bolted or soldered joints for these conductors do not demonstrate high reliability in practice.

Keywords: *resistance welding, strong magnetic fields, specific electrical conductivity, mechanical properties, microstructure.*

References:

1. Škamat et al. *Mokslas – Lietuvos Ateitis* **8(6)** p. 609–614 (2017)
2. Jiang et al. *IEEE Transactions on Applied Superconductivity* **26(4)** p. 1–6 (2016)

P7. Green Synthesis of Silver Nanoparticles from Fermented Origanum vulgare Extract and Their Antimicrobial, Antioxidant Activity and Phytochemical Composition

Syeda Hijab Zehra, Aistė Balčiūnaitienė, Jonas Viškelis

Institute of Horticulture, Lithuanian Research Centre for Agriculture and Forestry, 54333 Babtai, Lithuania
hijab.zehra@lammc.lt

Nanotechnology is the most advanced and diverse field with multidirectional applications in the twentieth century. Green silver nanoparticles (AgNPs) were synthesized using plant extract in aqueous form as bio-reducing and bio-capping agents. Due to their therapeutic potential applications, various metallic nanoparticles are extensively prone to use in nanomedicine. Silver nanoparticles are remarkable in their physical and chemical properties. This study aims to develop biosynthesized NPs made using fermented Origanum vulgare extract, having increased antioxidant and antimicrobial activities. Nanoparticles have a size range of 1–100 nm, specifically silver has high antimicrobial properties. The biosynthesized NPs were characterized by Transmission Electron Microscopy (TEM), Scanning Electron Microscopy-Energy-Dispersive Spectroscopy (SEM-EDS) techniques, and different spectrophotometric measurements. Prepared silver nanoparticles increase antimicrobial activity against Gram-negative and Gram-positive bacteria growth by applying the Kirby-Bauer disk diffusion test. The prominent increase in antioxidant activity is due to the phenolic compounds in Origanum vulgare extract. TEM analysis visually confirms the spherical shape and size of 10–20 nm. SEM-EDS was performed for green AgNPs and precise and uniform distribution. This research describes for the very first time the use of fermented Origanum vulgare for the preparation of AgNPs and proves an increase in antioxidant and antimicrobial activity with confirmatory analytical tests and calculations.

Keywords: *green synthesis; Origanum vulgare, silver nanoparticles, fermentation, phytochemical analysis, antibacterial activity, antioxidant activity.*

References:

1. C. Tyavambiza et al. *Nanomaterials* **11(5)** p. 1343 (2021)
2. V. Mansouriet et al. *Biomed. Pharmacother.* **141** p. 111875 (2021)
3. A. R. H. Mahmoud et al. *Toxicol. Environ. Health Sci.* **15(2)** p. 119–125 (2023)

SURFACE ENGINEERING AND NANOSTRUCTURES

P8 – P22

P8. Optical Characterization of Bismuth Sulfide Film Deposited on FTO Glass

Aistis Melnikas, Skirma Žalenkienė

Department of Physical and Inorganic Chemistry, Kaunas University of Technology, Lithuania
aistis.melnikas@ktu.edu

Bismuth sulfide is a widely used non-toxic semiconductor, popular for its band gap energy value of 1.3 eV. Coupled with FTO glass, it serves as an ideal choice for an optoelectronic device for solar cells and many more.

Our study focuses on the reaction between $Bi(NO_3)_3 \cdot 5H_2O$ and L-cysteine, an environment-friendly sulfur source, with the employment of EDTA-Na_2 as a chelating agent. The impact of EDTA-Na_2 on the particle size and dispersion can be explained by the coordination chemistry theory wherein EDTA-Na_2 initially coordinates with bismuth ions through its two amines and four carboxylates to form a stable ring structure $[Bi\text{-}EDTA]^-$ [1], thus the direct binding of Bi^{3+} with S^{2-} is prevented, making the reaction product more disperse. With the increasing temperature, Bi_2S_3 nuclei form gradually to make up crystals. The reaction takes place at 90ºC and is continuous for at least 8 hours, resulting in the formation of dark Bi_2S_3.

Precipitate is collected and dispersed in the solution of glycerol and anhydrous ethanol in 1:1 ratio. The suspension is later added to FTO glass and deposited by spin coating method for 60 seconds maintaining 2000 RPM.

Ultraviolet-visible (UV-Vis) spectroscopy in the 200–800 nm range using a Perkin Elmer Lambda 35 UV-Vis spectrometer was used to study the optical properties of the deposited bismuth sulfide film. Based on the obtained results, the band gap values of thin bismuth sulfide layers obtained by the Tauc diagram method were calculated.

Optical microscopy of thin bismuth sulfide layers was performed with an optical microscope Olympus SZX7 with a photo camera, magnification – x112. The acquired results were compared and discussed.

Keywords: *thin film, UV-Vis, bismuth sulfide.*

References:
1. L. Zeng et al. *Journal of Materials Chemistry B* **8(18)** p. 4093–4105 (2020)

P9. The Design and Manufacturing of High Diffraction Efficiency Gratings Based on Multi-Layer Dielectric Mirrors

Andrius Žutautas[1], Sigitas Tamulevičius[1,2], Tomas Tamulevičius[1,2]

[1]Institute of Materials Science, Kaunas University of Technology, K. Baršausko St. 59, LT-51423 Kaunas, Lithuania
[2]Department of Physics, Kaunas University of Technology, Studentų St. 50, LT-51368 Kaunas, Lithuania
andrius.zutautas@ktu.lt

The invention of the laser marked a giant leap in technology, unlocking a vast array of new applications of light. From everyday devices to military operations, lasers have become ubiquitous. This widespread interest has fuelled ongoing research and development, pushing the boundaries of laser technology in pursuit of even greater power, faster pulses, and innovative amplification methods and these advancements have opened doors to entirely new applications [1].

One of the most significant breakthroughs came with the development of chirped pulse amplification systems, which dramatically increased laser power output. These systems rely on diffraction gratings, specifically paired gratings that stretch and compress the laser pulse temporally and spatially before and after amplification to prevent damage to the gain medium [2]. Current research focuses on developing near-perfect diffraction efficiency gratings. This involves analysing various geometries using rigorous coupled wave analysis and then fabricating these structures on commercially available mirrors using techniques like deep reactive ion etching and electron beam lithography [3].

Keywords: *diffraction, diffraction efficiency, diffraction gratings, multi-layer dielectric mirror.*

References:

1. N. Bonod et al. *Advances in Optics and Photonics* **8(1)** p. 156–199 (2016)
2. D. Strickland et al. *Optics Communications* **56(3)** (1985)
3. S. Fu et al. *Optical Engineering* **60(2)** (2021)

P10. Development and Characterization of Hexylamine 2D WTe_2 Protective Coatings

Aris Jansons[1], Andrejs Terehovs[1], Darja Dolbe[1], Jevgenijs Gabrusenoks[2], Anatolijs Sarakovskis[2], Gunta Kunakova[1]

[1]Institute of Chemical Physics, University of Latvia, Jelgavas Street 1, LV-1004 Riga, Latvia
[2]Institute of Solid State Physics, University of Latvia, Ķengaraga Street 8, LV-1063 Riga, Latvia
aris.jansons@lu.lv

2D transition metal dichalcogenides (TMDCs) are promising for applications in variety of optical and electronic devices. One of 2D TMDCs which has recently attracted a lot of attention, is tungsten ditelluride (WTe_2). Its giant magnetoresistance and exotic topological insulator properties makes it a suitable candidate for development of magnetic memory devices, magnetic sensors and spintronics [1].

Majority of applications rely on stable charge transport characteristics, however, 2D WTe_2 rapidly oxidizes upon exposure to ambient environment, and extra capping layer preserving intrinsic electronic properties of WTe_2 has to implemented [2].

One of the most promising methods for forming passivation layers on several 2D TMDCs is based on deposition of linear alkylamines [3], but it has been verified only on exfoliated flakes, and all steps including fabrication of 2D structures being performed in glovebox with controlled inert atmosphere. However, for CVD or MBE grown 2D WTe_2, all-in-glovebox sample fabrication procedures are often challenging to ensure.

Here we show how to implement coating procedure of n-hexylamine passivation layer ex-situ on CVD grown WTe_2. Fabricated n-hexylamine passivated CVD grown 2D WTe_2 samples were studied via Raman spectroscopy and further implemented into devices to study the charge transport.

Obtained Raman spectra and magnetotransport measurements at low temperatures show that n-hexylamine coating method can be used efficiently to protect CVD-grown 2D WTe_2 from rapid degradation under ambient conditions, allowing the fabrication of WTe_2 based nanoelectronic devices on site in any laboratory without need for glovebox with low O_2 and H_2O levels, designated specially for application of linear alkylamines.

***Keywords**: 2D TMDC, WTe_2, hexylamine, charge transport carrier measurements.*

References:

1. M. Ali *et al. Nature* **514(7521)** p. 205–208 (2014)
2. J. Woods et al. *ACS applied materials & interfaces* **9(27)** p. 23175–23180 (2017)
3. S. Cong *et al. PNAS* **116(42)** p. 20844–20849 (2019)

P11. Site Selective Growth of 2D Tungsten Ditelluride

Darja Dolbe[1], Andrejs Terehovs[1], Martins Zubkins[2], Gatis Mozolevskis[2], Gunta Kunakova[1]

[1]Institute of Chemical Physics, University of Latvia, Jelgavas St. 1, Riga, Latvia
[2]Institute of Solid State Physics, University of Latvia, Ķengaraga St. 8, Riga, Latvia
darja.dolbe@lu.lv

Two-dimensional (2D) materials have become forefront in the development of nanoelectronic devices and for fundamental studies of new phenomena. Recently discovered higher order topological insulator states in few-layer structures [1], quantum spin Hall insulator state [2] and superconductivity [3] in monolayer tungsten ditelluride (WTe_2) highlight it as one of the most prominent 2D materials. However, controlled growth of 2D WTe_2 remains a challenging task due to the low bonding energy of Te and the high melting points of W precursors. Commonly used chemical vapour deposition (CVD) growth lacks control over nucleation sites on the substrate, yielding highly nonuniform distribution of 2D WTe_2 materials with different thicknesses. One promising route is to use substrates with predefined nucleation sites, a studied approach for several classical 2D materials, but not for the growth of WTe_2.

Here, we have developed a site selective synthesis approach for obtaining high-quality, uniformly distributed 2D WTe_2 structures on insulating substrates. This has been achieved by introducing precursor arrays fabricated via etching of sputtered WO_3 thin films and further functionalizing them prior CVD growth in a two-zone tube furnace. The obtained WTe_2 structures have been used to fabricate arrays of devices for charge transport measurements.

Our results show that site selective CVD growth of WTe_2 is a promising method for obtaining arrays of mono- and few-layer structures on insulating substrates, including hexagonal boron nitride, which is particularly important for fundamental studies of unconventional electronic properties.

Keywords: *CVD, tungsten ditelluride, site-selective.*

References:

1. Y. B. Choi et al. *Nat. Mater*. **19 (9)** p. 974–979 (2020)
2. S. Tang et al. *Nature Phys*. ***13* (7)** p. 683–687 (2017)
3. V. Fatemi et al. Science ***362 (6417)*** p. 926–929 (2018)

P12. The Influence of Spike Size on the Linear and Nonlinear Optical Properties of Gold Nanourchins

Domantas Peckus[1], Fatima Albatoul Kasabji[2], Maziar Moussavi[1], Loic Vidal[2], Asta Tamulevičienė[1], Arnaud Spangenberg[2], Karine Mougin[2], Sigitas Tamulevičius[1]

[1]Institute of Materials Science, Kaunas University of Technology, K. Baršausko St. 59, LT-51423 Kaunas, Lithuania
[2]Institut de Science des Matériaux de Mulhouse IS2M UMR 7361, 15 rue Jean Starcky, F 68100 Mulhouse, France
domantas.peckus@ktu.lt

Plasmonic metallic nanoparticles have shown great promise due to their unique optoelectronic applications like photocatalysis, medicine, etc. So far, the best analyzed plasmonic properties are of gold and silver nanoparticles of shapes like spheres, nanorods, nanocubes, and bipyramids. Due to recent advances in chemical synthesis methods, gold nanoparticles of new shapes have been synthesized, such as nanourchins, nanostars, and nanoflowers, that in general have the core of the sphere with some outgrowths such as spikes or petals (fig. 1). To our knowledge, these outgrowths dramatically change the plasmonic properties of nanospheres, but it is not understood completely [1].

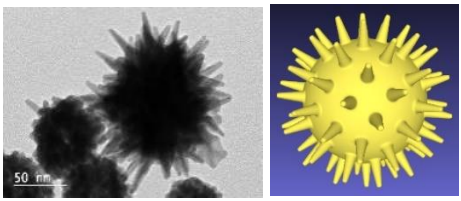

Fig. 1. TEM image and model of Au nanourchins

In our work, we analyze nanoparticles of gold nanourchins. The main objective of the research was to systematically study how the size of spikes of nanourchins changes their plasmonic properties. For this, we used gold nanospheres and nanourchins with different lengths of spikes. We analyze how the size of the spikes influences the steady-state absorption spectra and transient absorption dynamics. The results show that Au nanourchins with very short spikes have optical properties quite similar to Au nanospheres while long spikes change optical and plasmonic properties significantly (Au nanourchins with short spikes has an absorption spectrum at 500–700 nm while Au nanourchins with long spikes has an absorption peak at 500–1000 nm).

Acknowledgements: The studies were performed within the NANOTRAACES project carried out under the M-ERA.NET 2 scheme, MERANET-22-2 and co-funded by the Research Council of Lithuania.

Keywords: *transient absorption spectroscopy, gold nanourchins, spikes of Au nanourchins.*

References:

1. D. Issaad et al. *J. Phys. Chem. C* **121** p. 18254−18262 (2017)

P13. Features of Using the Laser GRBL Control Program for Forming Point Grating Images

Algirdas Lazauskas, Virgilijus Minialga, Erika Rajackaitė, Andrius Žutautas

Institute of Materials Science, Kaunas University of Technology,
K. Baršausko St. 59, LT-51423 Kaunas, Lithuania
virgilijus.minialga@ktu.lt

Images formed from surface-relief diffraction grating points are used for decorative decoration and protective marking purposes. The characteristic of the formed pictures or signs is that, depending on the illumination of the surface and the direction of observation, the predominant color of the light reflected from the selected image point changes.

Forming such images from relatively fine micrometric dots presents technological challenges.

Device assemblies must maintain mechanical stability and repeatability with micrometer part tolerances. An important part is the quality of the control program (code) of all nodes of the device.

Due to errors in the control program, the correct operation of the dot grid imaging device becomes unsatisfactory. Experience has shown that it is possible to adapt control programs for laser engraving and cutting machines. Several groups of such programs have been created. We adapted the Laser GRBL program of moderate complexity [1].

Using GRBL Laser v.4.9.4 program in the device we had to change the controllers for the stepper motors. When debugging the program itself, it was chosen that the X and Y channels will control the stepper motors that move the tables in the x and y directions. The Z channel was selected for the rotation control of the diffraction grating optics.

In order to obtain the point structure, a code forming program was created that divides the illumination of the laser light beam into points, instead of leaving continuous lines in the image forming plane. The volume of code compiled in this way increased, but the quality of the images improved significantly.

The following parameters can be changed during code generation:

- distance between points;
- duration of illumination;
- the power of illumination;
- table movement speed between points;
- the section of the turning angles of the grating;
- color coding system;
- swap the left and right sides of the picture with little effort.

Keywords: *diffraction grating, point grating, laser engraving.*

References:

1. Laser GBRL – free laser engraving - https://lasergrbl.com/

P14. Electrochemical Sensor Based on MXenes for Accurate Detection of Lead and Cadmium Ions

Ilya Navitski[1], Šarūnas Žukauskas[1], Alma Ručinskienė[2], Arūnas Ramanavičius[1,3]

[1]Department of Nanotechnology, State Research Institute Center for Physical Sciences and Technology (FTMC), Sauletekio Ave. 3, LT-10257 Vilnius, Lithuania
[2]Department of Electrochemical Material Science, State Research Institute Center for Physical Sciences and Technology (FTMC), Sauletekio Ave. 3, LT-10257 Vilnius, Lithuania
[3]Department of Physical Chemistry, Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University (VU), Naugarduko St. 24, LT-03225 Vilnius, Lithuania
ilya.nov42@gmail.com

A vast amount of lead and cadmium waste has accumulated over centuries due to their common use in industry. This accumulated waste poses a serious hazard to human health through groundwater contamination. Therefore, it is necessary to develop quick and affordable techniques for accurately detecting lead and cadmium ions in water samples.

We have designed an electrochemical sensor capable of identifying lead and cadmium ions in aqueous solutions by utilizing their unique interaction with pure delaminated MXenes. The sensor was fabricated using the drop-casting method, applying three layers of a MXene-Nafion mixture onto the working electrode's surface. Differential pulse voltammetry (DPV) and cyclic voltammetry (CV) were employed to evaluate the sensor's performance, focusing on factors such as sensitivity and limit of detection (LOD).

The developed sensor demonstrated remarkable selectivity for lead ions, low LOD values for both cadmium and lead ions, and the ability to identify both directly in samples without requiring a lengthy preparatory procedure. This research lays the groundwork for future development of MXene-based electrochemical sensors.

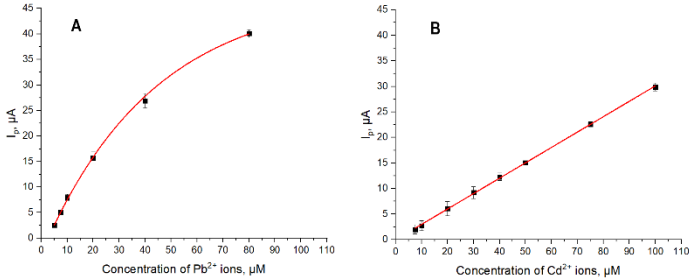

Fig. 1. Lead **(A)** and cadmium **(B)** ion concentration curves determined by differential pulse voltammetry using a GCE/MXene+Nafion electrode

Keywords: *MXenes, electrochemical sensor, lead detection, cadmium detection.*

P15. Electret Templates for Metal-insulator Surface Structures

Maksym Barabash[1,2], Dmytro Gryn'ko[1], Roman Lytvyn[1], Anton Sezonenko[1], Vladyslav Martynchuk[1], Anastasiia Kolesnychenko [1], Maryna Romashkina [1], Bogdan Pysarevskyi [1], Yeva Boboshko[1,2]

[1]Technical Center N.A.S. of Ukraine, Pokrovs'ka St. 13, UA-04070 Kyiv, Ukraine
[2]National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", 37 Beresteiskyi Ave., UA-03056 Kyiv, Ukraine
mbarabash@nasu.kiev.ua

Strong spatially inhomogeneous electric fields near the template surface can be formed by the electro-photographic method. This method provides predictable topology of electric field near a photoconductive thin-film object using inhomogeneous light field, for example interference one. In electrostatic templates, the inhomogeneity of electric field can be caused by the surface relief (at a uniform surface charge density), or modulated surface charge density, or modulated volume charge. The latter one is the template of electret type. Such templates longer preserve their properties and can be used multiple times.

Under exposure to light, photogeneration of current carriers occurs, and photoconductivity appears in a charged nanocomposite film [1]. The photoconductivity current density is modulated by the intensity of exposing light field. Photocurrents decrease the potential on the film surface. After the end of the exposure, non-uniformly distributed charges appear on the surface and in the volume of the film. The surface charge density is modulated by the exposing light field. Spacially modulated field of surface and volume charges can deform the film during its softening and form a stable relief and stable spatially distributed charge after solidification.

In our experiments, the time of surface relief formation was several tenths of a second. The reproducibility of parameters was provided by automatic hologram registration with a control module [1].

When the photocurrent flows through the film, charge carriers are trapped by deep traps, and a localized charge modulated by the exposing light field appears. As a result, volume charge forms. The probability of carrier trapping is determined by the density and energy parameters of deep traps which in our experiments formed, apparently, during vacuum deposition of the nanocomposite. The density of the electric charge localized in the film is modulated proportionally to the intensity of the exposing light field and, therefore, has the same topology as the relief.

A new approach to the formation of electret templates by the electro-photographic technique is proposed. An electret template of about 1 cm^2 area was produced by the electro-photographic method when a film of nanocomposite photoconductor was exposed to the light field of a planar hologram.

Keywords: *template, electrostatic relief, hologram.*

References:

1. M. A. Zabolotnyi at al. *Nanosistemi, Nanomateriali, Nanotehnologii* **21(2)** p. 261–271 (2023)

P16. Reduction of Gold Thin Film Reflectance on Quartz Crystal Resonators via Femtosecond Laser-Processing

Mantas Mikalkevičius[1], Martin Hruška[2], Joris More Chevalier[3], Fitl Premysl[2,3], Martin Vrňata [2], Michal Novotný[2,3], Asta Tamulevičienė[1,4], Tomas Tamulevičius[1,4]

[1]Institute of Materials Science, Kaunas University of Technology, K. Baršausko St. 59, LT-51423 Kaunas, Lithuania
[2]University of Chemistry and Technology, Technicka 5, CZ16628, Prague 6, Czech Republic
[3]Institute of Physics, Czech Academy of Sciences, Na Slovance, 1999/2, CZ182 21, Prague 8, Czech Republic
[4]Department of Physics of Kaunas University of Technology, Studentų St. 50, LT-51368 Kaunas, Lithuania
mantas.mikalkevicius@ktu.lt

Quartz crystal microbalance (QCM) sensors are used in telecommunications and integrated circuits for generating a stable clock frequency from kHz to MHz due to the inverse piezoelectric effect. There is a shift in resonant frequency when atoms or molecules are adsorbed on their electrodes meaning QCMs can be used as effective sensors, for example for gas detection [1]. Adsorption of molecules to be detected requires elaborated surfaces where black metals are highly beneficial.

In this work, Yb:KGW 1030 nm wavelength femtosecond laser was used for patterning QCR gold films with laser-induced periodical surface structures (LIPSS). The laser beam was scanned in straight lines over the gold electrodes with a galvanometer scanner and a telecentric f-Theta lens varying power and pulse density.

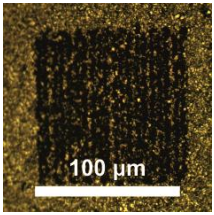

Fig. 1. Optical microscope image of laser-processed gold surface

Once power exceeded 136 mW, LIPSS structures started to form and increasing the power further till 205 mW made the thin film darker. Black electrodes will be later tested for gas sensing experiments.

Keywords: *femtosecond laser, gold thin films, quartz resonators, black metals.*

References:

1. C. Zhang *et al. Measurements* **124(3)** p. 286–290 (2018)
2. M. Hruška *et al. Applied Surface Science* **647** p. 158618 (2024)

P17. Use of Environmentally Friendly and Biodegradable Organic Materials in Granular Fertilizers

Odeta Pocienė, Rasa Šlinkšienė

Department of Physical and Inorganic Chemistry, Kaunas University of Technology, Radvilėnų Rd. 19, LT-50254 Kaunas, Lithuania
odeta.pociene@ktu.lt

Fertilizers, crucial for maximizing crop yields, are undergoing scrutiny due to their environmental impact and health concerns. In order to solve these problems, efforts are being made to use less concentrated mineral fertilizers, replacing them with fertilizing products made from environmentally friendly raw materials. Organic wastes such as plant residues, plant and animal by-products (bone meal, fish meal), food scraps, etc., which are rich in nutrients, are perfect for composting or other forms of processing into fertilizers [1,2]. According to the World Bank, global waste generation is expected to increase by 70% by the year 2050 [3]. Therefore, recycling wastes into fertilizer is often a part of broader initiatives to promote a circular economy and reduce the environmental impact of waste disposal.

In this research, different solid and liquid waste from food industry was used to granulate organic biofertilizers with a rotary drum granulator. Different raw materials as buckwheat biomass (BBM), buckwheat hulls (BH), buckwheat hull ash (BHA), bone meal (BM), molasses solution (MS), and beaten eggs (BE) were mixed in various ratios and granulated by wet granulation with a drum granulator to obtain spherical granules. Different amounts of liquid binder (MS or BE) were used to improve the agglomeration of organic raw materials. Eight different fertilizer compositions were created:

20% BHA + 40% BH + 40% BBM + BE
20% BHA + 40% BH + 40% BBM + MS
40% BHA + 30% BH + 30% BBM + BE
40% BHA + 30% BH + 30% BBM + MS
20% BHA + 20% BH + 20% BBM + 40% BM +BE
20% BHA + 20% BH + 20% BBM + 40% BM +MS
40% BHA + 10% BH + 10% BBM + 40% BM +BE
40% BHA + 10% BH + 10% BBM + 40% BM +MS

Using standardized fertilizer testing methods, it was found that the biofertilizers produced by the drum granulator meet the requirements for bulk fertilizers, as they are rich in plant nutrients.

Keywords: *fertilizers, organic wastes, binder, granulation.*

References:

1. K. W. Chew et al. *Sustainability* **11** p. 2266 (2019)
2. S. Stankowski et al. *Agronomy Research* **19(4)** p. 1999–2012 (2021)
3. The World Bank. Global Waste to Grow by 70 Percent by 2050 Unless Urgent Action is Taken: *World Bank Report* (2018)

P18. Research of the Catalyst Chamber and Bed Properties of a Monopropellant Rocket Thruster

Paulius Baronas[1], Sigitas Kilikevičius[2], Inga Morkvėnaitė-Vilkončienė[3]

[1]Faculty of Mechanical Engineering and Design, Kaunas University of Technology, K. Baršausko St. 59, LT-51423 Kaunas, Lithuania
[2]Department of Electrical Engineering, Vilnius Gediminas technical university, Plytinės St. 5, LT-10105 Vilnius, Lithuania
pauliusbaronascv@gmail.com

Chemical monopropellant propulsion systems are shifting towards non – toxic, green compounds, such as ammonium dinitramide, high-test peroxide and hydroxylammonium nitrate [1,2]. These fuels require a catalyst to initiate and sustain the decomposition reaction, which must be applied on a stable, high surface area matrix [3]. For this reason, it was proposed to make a stable, high surface area, dense, heat tolerant catalytic bed, using high-pressure particle packing method from the sphere of chromatography.

Therefore, this work aims to evaluate the feasibility of such method and compare the suggested packing method to existing one. In addition, several configurations of the proposed packing method were analysed and discussed. The experiments were carried out by preparing several test and control samples with different size of Al_2O_3 particles as well as different preparation approaches. Test samples were packed using high pressure pump, while control samples were packed with free-falling granules. Afterward, the backpressure of all samples was measured at different flow rates and compared.

It was determined that 600–1200 μm particles were the most suitable ones to be used as catalyst support, since more reasonable backpressure values were achieved. Additionally, it was found that the mixture of H_2O and sodium dodecyl sulphate was the most suitable solvent to disperse the particles in, due to favourable sedimentation and agglomeration effects.

Keywords: *propulsion, catalyst chamber, catalyst bed, monopropellant.*

References:

1. W. M. Marshall et al. *49th AIAA/ASME/SAE/ASEE Joint Propulsion Conference* **1** PartF p. 1–13 (2023)
2. R. Amrousse et al. *In Combustion and Flame* **176** p. 334–348 (2017).
3. A. Cervone et al. *In Collection of Technical Papers - AIAA/ASME/SAE/ASEE 42nd Joint Propulsion Conference* **11** p. 8786–8796 (2006)

P19. Self-Assembled Monolayers on Screen-Printed Electrodes: Formation and Evaluation

Simona Raišytė[1], Viktorija Liustrovaitė[2], Arūnas Ramanavičius[1,2]

[1]Department of Nanotechnology, State Research Institute Center for Physical and Technological Sciences (FTMC), Saulėtekio Ave. 3, LT-10257 Vilnius, Lithuania
[2]NanoTechnas – Center of Nanotechnology and Materials Science, Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Naugarduko St. 24, LT-03225 Vilnius, Lithuania
simona.raisyte@ftmc.lt

In modern society, with a growing interest in the impact of the environment on human beings and their biological processes, scientists are working to develop more efficient, rapid, and precise methods to understand such events. One of these methods is the development of electrochemical systems (biosensors). The development of biosensors begins with modification of the working electrode surface. The electrode needs a functionalization procedure which includes the deposition of organic molecules that demonstrate specific recognition capabilities, enabling the following binding of analytes. The formation of a self-assembled monolayer (SAM) is a common technique for modifying the electrode surface. The terminal groups of the constituent molecules in the SAM have a significant impact on its functionality and structure, determining its suitability for biosensor development [1,2].

The impact of the self-assembled monolayer structure and its constituent molecules on the physical characteristics of the screen-printed electrode (SPE) surface has been studied using square wave voltammetry (SWV) and electrochemical impedance spectroscopy (EIS).

The effective formation of self-assembled monolayers has been confirmed by an increase in charge-transfer resistance and a decrease in current density compared to bare SPE results. These findings indicate that established electrochemical systems have the potential to serve as a basis for the development of biosensors.

Keywords: *self-assembled monolayer, biosensor, square wave voltammetry, electrochemical impedance spectroscopy, screen-printed electrode.*

References:

1. V. Liustrovaite et al. *Journal of Electrochemistry Society* **169** p. 037523 (2022)
2. M. Drobysh et al. *Science of the Total Environment* **908** p. 168154 (2024)

P20. Advancing SEIRA Spectroscopy for *in situ*: Fiber-Based Detection of Naphthalene with Ag-PVP Nanoparticles

Sonata Adomaviciute-Grabusove[1], Olga Bibikova[2], Tatiana Sakharova[2], Viacheslav Artyushenko[2], Valdas Sablinskas[1]

[1]Institute of Chemical Physics, Vilnius University, Sauletekio Ave. 3, LT-10257 Vilnius, Lithuania
[2]Art photonics GmbH, Rudower Chaussee 46, 12489 Berlin, Germany
sonata.adomaviciute@ff.vu.lt

Surface Enhanced Infrared Absorption (SEIRA) spectroscopy has evolved by utilizing mainly metal nanostructures for signal enhancement. Specifically, researchers have demonstrated the tuning of metal plasmon resonance to the IR range through dipolar interactions in nano-antennas and nanoshells [1]. Despite advancements, SEIRA application in real-life settings remains complex. Our method addresses this challenge by utilizing AgCl/AgBr optical fibers within SEIRA spectroscopy. The SEIRA achievement involves the deposition of PVP-coated silver nanoparticles onto the fiber surface, facilitated by the interaction between PVP and AgCl/AgBr fiber surface. SEM images confirm the successful assembly of Ag-PVP nanoparticles on the PIR-fiber loop (approximately 50 ± 10 nm). These silver structures on silver halide fiber loop significantly enhance the infrared absorption signal of proximal molecules, thus enabling effective SEIRA detection.

Our innovative fiber-based SEIRA measurements have demonstrated the capability to detect naphthalene directly in water at concentrations as low as 50 µM, under *in situ* conditions. The findings also indicate that the interaction between naphthalene and the Ag-PVP nanoparticles is characterized by physical adsorption rather than covalent bonding. This advancement in surface engineering and nanostructure design marks a significant step forward in the practical application of the SEIRA technique, especially for the detection of environmentally critical, low-solubility toxic compounds like naphthalene.

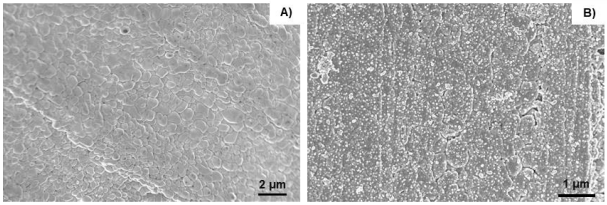

Fig. 1. SEM images SEM images of PIR-fiber loops without nanoparticles (A) and with the deposited Ag PVP nanoparticles (B)

Keywords: *SEIRA, ATR, ATR sensor, fiber, silver nanoparticles, silver halide.*

References:

1. S. Tian et al. *Nano Lett*. **17(8)** p. 5071–5077 (2017)

P21. A New Electrochemical Sensor for Lithium Hexafluorophosphate Detection

Wejden Gongi[1], Jerome Launay[2], Karine Mougin[1], Delphine Faye[3]

[1]Institut de Science des Matériaux de Mulhouse (IS2M), CNRS Mulhouse, France
[2]Laboratoire d'analyse et d'architecture des système, CNRS Toulouse, France
[3]Centre national d'études spatiales, CNES, Toulouse
wejden.gongi@uha.fr

Lithium-ion batteries (LIBs) represent the largest share of the electrical battery storage of our modern society and are considered to be a valid technology during the next twenty years for plug-in hybrid applications and electric vehicles. One issue in conversion of chemical into electrical energy is that damages such as overcharging lead to fatal composition changes and leaks outside the battery. To respond to the massive societal increasing needs battery safety issues have to evolve to overcome these limitations.

This study presents the development of a new sensor based on gold nanoparticles for detecting lithium during battery leakages. An experimental plan involving two factors, pH and gold concentration, was developed to achieve a dendritic shape of nanosensors; at this level, temperature and the time of electroplating were also optimized. The dendritic shape was further confirmed through SEM characterization. Finally, the sensor's ability to detect lithium hexafluorophosphate was investigated using both cyclic voltammetry and impedance spectroscopy techniques using various electrolytes commonly used in the batteries industry.

Results showed that the sensor has successfully detected lithium in acetonitrile across a range of concentrations using cyclovoltammetry analysis, while impedance spectroscopy results indicated detection capabilities in methyl acetate up to a very low concentration.

However, further research is needed to explore the sensor's potential for detecting lithium in gaseous states.

Keywords: *sensor, dendritic shape, cyclovoltammetry, impedance spectroscopy, Lithium.*

P22. Development of Technology for Integrating Holograms into the Surface of Plastic Products

Erika Rajackaitė, Indrė Danisevičienė, Andrius Žutautas, Pranas Narmontas

Institute of Materials Science, Kaunas University of Technology,
K. Baršausko St. 59, LT-51423 Kaunas, Lithuania
erika.rajackaite@ktu.lt

Incorporating holograms or other light-diffracting surface relief patterns onto molded plastic components ensures product authentication. Developing mass replication techniques for plastic articles with surface microstructures via injection or blow molding using a unitary mold is crucial. These microstructures can be created by attaching metal film replicas of holograms to the model, by electrodeposition, or directly forming the hologram on the model's surface with photosensitive materials [1–3]. Our research involves producing diffractive elements from a unique graphic design to a final product with security elements, utilizing the full hologram production cycle: mathematical modeling, dot-matrix recording, silver vacuum evaporation, electrochemical nickel master deposition, and recombination. The configuration of diffraction structures and hologram properties were thoroughly studied to improve the replication of surface relief holograms on molded plastic parts, ensuring authenticity and meeting global production standards.

Keywords: *diffraction grating, authentication, hologram, replication.*

References:

1. X. Wang et al. *Optics and Laser Technology* **135** p. 106687 (2021)
2. Dan Chen et al. *Advanced Materials* **34** p. 2200903 (2022)
3. Yangxi Fu et al. *Scientific Reports* **10** p. 22428 (2020)

ELECTRONIC AND OPTICAL MATERIALS

P23 – P47

P23. Emission Efficiency Investigation of GaAsBi-based VECSEL

Aistė Butkutė[1], Aivaras Špokas[1], Andrea Zelioli[1], Augustas Vaitkevičius[1,2], Renata Butkutė[1], Evelina Dudutienė[1]

[1]Department of Optoelectronics of SRI Cente for Physical Sciences and Technology, Saulėtekio Ave. 3, LT-10257 Vilnius, Lithuania
[2]Institute of Photonics and Nanotechnology, Faculty of Physics, Vilnius University, Saulėtekio Ave. 3, LT-10257 Vilnius, Lithuania
aiste.butkute@ftmc.lt

Vertical-External-Cavity Surface-Emitting Lasers (VECSELs) are versatile semiconductor lasers that offer unique advantages in terms of tunability, efficiency, output power and can be applied in optical telecommunications, spectroscopy [1].

This work presents detailed optical study of GaAsBi/GaAs multiple quantum well (MQW) structures, which represent optimized growing method for active area for VECSELs, where the pairs of QWs are placed periodically to match the antinodes of the optical standing wave in order to have thinner structures with higher homogeneity and enhanced PL intensities.

In this work optical properties of GaAsBi structures were investigated using temperature dependent photoluminescence. The internal quantum efficiency (IQE) was evaluated by employing absolute IQE measurement with an integrating sphere [2], relative temperature dependent and excitation power dependent methods, also, additional non-radiative recombination mechanism – trap-assisted Auger recombination [3] was considered. All the emission efficiency estimation techniques were compared and the most reliable method has been selected.

This quantitatively assessed emission efficiency allows to compare structures grown and characterized in different laboratories and evaluate the amount of non-radiative recombination.

Acknowledgements: Work was supported by Research Council of Lithuania, Grant. No. S-LLT-23-3 and Grant. No. S-PD-22-7.

Keywords: *GaAsBi, VECSEL, quantum well, photoluminescence, emission efficiency.*

References:

1. K. S. Kim et al. *IEEE Photonics Technology Letters* **19(20)** p. 1655–1657 (2007)
2. S. Leyre et al. *Review of Scientific Instruments* **85** p. 123115 (2014)
3. A. C. Espenlaub et al. *Journal of Applied Physics* **126** p. 184502 (2019)

P24. GaAsBi: From MBE Growth to NIR Emitters

Aivaras Špokas, Andrea Zelioli, Andrius Bičiūnas, Mindaugas Kamarauskas, Aurimas Čerškus, Bronislovas Čechavičius, Evelina Dudutienė, Renata Butkutė

Center for Physical Sciences and Technology, Saulėtekio Ave. 3, LT-10257 Vilnius, Lithuania
aivaras.spokas@ftmc.lt

GaAsBi has emerged as a material capable of covering most of the second near infrared (NIR-II) region, while also offering a variety of advantageous properties in rapid bandgap reduction (up to 90 meV/%$_{Bi}$) [1], decreased non-radiative losses [2], and a temperature insensitive emission wavelength.

In the current work we focus on growing optimal GaAsBi quantum well structures using MBE and fabricating NIR emitters (light emitting diodes and laser diodes) oriented at biosensing applications. All devices have been grown on GaAs substrates buffered by AlAs sacrificial layer, that is necessary for substrate removal, which in turn allows for integration onto a silicon-based platform. Devices were fabricated on p- and n-doped GaAs substrates and by employing different designs of polarity; detailed protocols on technological procedures and growth challenges will be presented. Peak emission wavelength for the light emitting diode was registered at 1070 nm in room temperature. Furthermore, temperature dependent measurements showed a temperature insensitive operation. Two laser diode structures were grown and processed to measure their lasing spectra. Room temperature lasing was recorded at 1003 nm and 1142 nm.

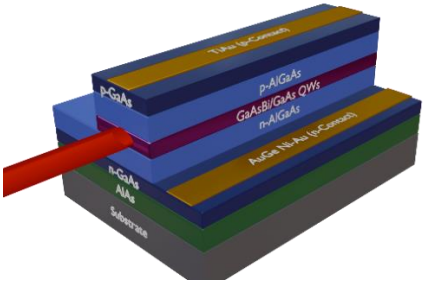

Fig. 1. Schematic of a FP edge emitting laser diode

Acknowledgements: This work was supported by the Research Council of Lithuania under Contract No S-LLT-23-3; project "Development of A3B5-Bi Nanostructure Based Double-Wavelength Microlaser Technology for NIR Sensing Applications".

Keywords: *molecular beam epitaxy, laser diodes, bismide, quantum well.*

References:

1. K. Alberi et al. *Appl. Phys. Lett*. **91** p. 10–13 (2007)
2. S. Francoeur et al. *Appl. Phys. Lett.* **82** p. 3874–3876 (2003)

P25. Modulating Luminescence and Charge Transporting Properties of Dibenzo[*a,c*]imidazophenazine-based Emitters by Changing the Donor Substituents

Aliyu Mohammed Hamisu, Viktorija Andruleviciene, Matas Guzauskas, Juozas Vidas Grazulevicius

Kaunas University of Technology, Department of Polymer Chemistry and Technology, Kaunas, Lithuania
hamisu.mohammed@ktu.edu

The domain of purely organic emitters for light production in organic light-emitting diodes (OLEDs) remains a research theme of continuing interest, attributable to the efficient harvesting of non-emissive triplet excitons [1–3]. Of particular interest are emitters exhibiting thermally activated delayed fluorescence (TADF) and room temperature phosphorescence (RTP) emission. TADF emitters feature efficient exciton up-conversion from the dark triplet states to radiative singlet states through reverse intersystem crossing mediated by small singlet-triplet energy splitting [4–6]. In contrast, RTP emitters convert triplet excitons populated at triplet states through intersystem crossing to a long-lived radiative deactivation to the ground states mediated by efficient spin-orbit coupling [7].

Herein, a series of donor-acceptor-donor (D-A-D) type emitters were synthesized by coupling the dibenzo[*a,c*]imidazophenazine-based acceptor with various donors. Under certain conditions, compounds demonstrated either TADF, RTP or a combination of both emissions. Consequently, the compound containing phenothiazine moiety revealed surprisingly high photoluminescence quantum yield in vacuum, reaching 86% for the molecular dispersion in polymer matrix and 79% for the solid film. Furthermore, the D-A-D type compounds showed both hole and electron mobilities, exceeding 10^{-3} cm^2/Vs at high electric fields. The obtained results show that the synthesized dibenzo[*a,c*]imidazophenazine-based compounds are especially promising for the development of efficient OLEDs.

Keywords: *OLEDs, TADF, RTP, charge transport, organic emitter.*

References:

1. G. Zhao et al. *Angewandte Chemie International Edition* **61** p. e202212861 (2022)
2. G. Meng et al. *Nature Communication* **14** p. 2394 (2023)
3. Madayanad Suresh et. al. *Advanced Functional Material* **30** p. 1908677 (2020)
4. S. Y. Lee et. al. *Advanced Materials* **28** 4019–4024 (2016)
5. G. Méhes et. al. *Angewandte Chemie International Edition* **51** p. 11311–11315 (2012)
6. K. Goushi et. al. *Nature Photonics* **6** p. 253–258 (2012)
7. C. Chen Kenry et. al. *Nature Communication* **10** p. 2111 (2019)

P26. Magnetotransport Studies of CVD Synthesized Tungsten Ditelluride 2D Crystals

Andrejs Terehovs, Aris Jansons, Agnese Spustaka, Gunta Kunakova

Institute of Chemical Physics, University of Latvia, Jelgavas St. 1, Riga, Latvia
andrejs.terehovs@lu.lv

Tungsten ditelluride (WTe_2) possesses a variety of unconventional electronic properties, such as the type-II Weyl semimetal phase in bulk, 2D topological insulator, and tunable superconducting state in monolayer materials. For studies of WTe_2 aimed for future applications in electronic devices that take advantage of these exotic properties, the development of scalable growth methods on insulating substrates is crucial. So far, chemical vapor deposition (CVD) is one of the main methods for producing 2D WTe_2 structures. However, charge transport characteristics, such as mobility and carrier density, strongly depend on the growth conditions and additives used to reduce the tungsten precursor's melting point. To investigate the impact of growth parameters on charge transport characteristics, and ultimately produce 2D materials of comparable quality to those from exfoliated flakes, extensive charge transport characterization directly on the growth substrate, eliminating the extra step of structure transfer, would be needed. So far, the majority of the reported data presents magnetotransport studies on exfoliated flakes, but data available on transport in CVD-grown WTe_2 materials directly on the growth substrate is very limited.

In this study, we have investigated magnetotransport in CVD-grown 2D WTe_2 crystals directly on the growth substrate. The substrates used were Si/SiO_2, Si/SiO_2 with exfoliated h-BN flakes, and Si/SiO_2 with monolayer h-BN. The fabricated 2D WTe_2 on these substrates was then implemented into Hall bar devices using electron beam lithography followed by contact metallization. Magnetotransport measurements were conducted in PPMS-Dynacool9T cryostat. The obtained magnetotransport data for 2D WTe_2 grown on various substrates have been correlated with the CVD growth parameters.

Keywords: *CVD, tungsten ditelluride, magnetotransport.*

P27. New Anthracene and Alkoxycarbazole-based Derivatives for TTA-OLEDs

Audrius Bucinskas[1], Pavel Arsenyan[2], Tien-Lung Chiu[3], Oleksandr Bezvikonnyi[1], Dmytro Volyniuk[1], Juozas Vidas Grazulevicius[1]

[1]Department of Polymer Chemistry and Technology, Kaunas University of Technology, K. Baršausko St. 59, LT-51423 Kaunas, Lithuania
[2]Latvian Institute of Organic Synthesis, Aizkraukles 21, LV-1006 Riga, Latvia
[3]Yuan Ze University, No. 135, Yuandong Road, Zhongli District, Taoyuan City, Taiwan
audrius.bucinskas@ktu.lt

It is still of high importance to find stable deep-blue emitters for commercial organic light-emitting diodes (OLEDs) used in future solid-state lighting and full-color displays. A huge number of phosphorescent or thermally activated delayed fluorescent (TADF) materials have been published up till today [1], but because of long-lived triplet excitons especially within the blue phosphorescent or TADF OLEDs and as a result, formed high energy excited states chemical decomposition of the chemical structure of emitter can be resulted and followed by the drastic decrease of device lifetime. To minimize the mentioned risk triplet–triplet annihilation (TTA) emitters which drive the fusion of low triplet energy excitons to produce high energy singlet excitons followed by generation of visual light photons can be employed in the device structure. TTA phenomenon allows to overcome maximum internal quantum efficiency limit of conventional fluorescence materials as in the case of TADF and phosphorescence materials [2]. Therefore, in the search of new stable TTA emitters, we developed novel compounds using anthracene and various alkoxy-carbazole derivatives which possess blue and green emission (470–533 nm) and photoluminescence quantum yield up to 85% in solutions and up to 29% in films. The main synthesis routes of new emitters and a comparison of their photophysical, thermal, and electrochemical characteristics together with theoretical chemistry support will be shown in the presentation.

Acknowledgements: This work was supported by the project of scientific cooperation program between Latvia, Lithuania and Taiwan (grant LV-LT-TW/2023) and Research Council of Lithuania (LMTLT), Agreement No S-LLT-22-4.

Keywords: *OLED, TTA, anthracene, carbazole.*

References:

1. H. Jiang et al. *ACS Materials Letters* **5(3)** p. 822–845 (2023)
2. X. Li et al. *Reports on Progress in Physics* **86(9)** (2023)

P28. Enhancement of Efficiency of Red Organic Light-emitting Diodes Based on a New Derivative of Phenazine and Diphenylamine by a Quantum Well Approach

Dmytro Volyniuk[1], Mariia Stanitska[2], Lilia Deva[1,2], Melika Ghasemi[1], Pavlo Stakhira[1], Juozas Vidas Gražulevičius[2]

[1]Kaunas University of Technology, Baršausko St. 59, 51423 Kaunas, Lithuania
[2]Department of Electronic Engineering, Institute of Telecommunications, Radioelectronics and Electronic Engineering, Lviv Polytechnic National University, Stepan Bandera St. 12, 79013 Lviv, Ukraine
dmytro.volyniuk@ktu.lt

Many high-tech applications require red and infrared light-emitting sources, including telecommunication, healthcare health monitoring, military equipment, medicine, sensing, optogenetics, etc. [1]. For instance, red and infrared light-emitting sources with emission wavelengths higher than 650 nm can solve problems caused by optical absorption, light scattering, and autofluorescence during the fluorescent probing of biological objects. Compared to inorganic counterparts, red organic light-emitting diodes (OLEDs) are preferable for healthcare applications due to their potential biocompatibility, flexibility, low-temperature processability and environmental friendliness. However, the eternal quantum efficiencies (EQEs) of red and infrared OLEDs are lower than those of OLEDs with blue or green electroluminescence [2]. The main reason is explained by the energy gap law. Thus, the red organic emitters with a narrow band gap (smaller than 1.9 eV) are characterised by the increased probability of non-radiative relaxation of excited states as the energy gap decreases [3]. This problem could be potentially resolved either by improving the design of red emitters or constructing new device structures for red OLEDs.

We have developed a narrow-band organic semiconductor that includes phenazine and diphenylamine moieties. In doping-free OLEDs, this compound demonstrated stable red electroluminescence at 609 nm across various electric fields. Using polaronic light-emitting layers, which are double layers-based heterostructures containing wide-band (diphenyl[4-(triphenylsilyl)phenyl]phosphine oxide) and narrow-band (the developed red emitter) organic semiconductors, this compound showed by relatively 63% higher EQE than that of doping-free OLEDs. The quantum well approach allowed the enhancement of efficiencies of red OLEDs based on the derivative of phenazine and diphenylamine.

Acknowledgements: This project has received funding from the Research Council of Lithuania (LMTLT), project QUANT, agreement no S-LU-24-8.

Keywords: *red electroluminescence, phenazine, diphenylamine, quantum well.*

References:

1. M. Vasilopoulou et al. *Nature Photonics* **15** p. 656–669 (2021)
2. Z. Zhao et al. *Luminescence* **39** p. e4657 p. 1–11 (2024)
3. Y.-C. Wei et al. *Nature Photonics* **14** p. 570–577 (2020)

P29. Novel Host Materials for Stable Blue Thermally Activated Delayed Fluorescence OLEDs

Domantas Berenis[1], Rita Butkutė[2], Gediminas Kreiza[1], Giedrius Puidokas[1], Vaida Jašinskaitė-Koženiauskienė[2], Karolis Kazlauskas[1]

[1]Institute of Photonics and Nanotechnology, Vilnius University, Saulėtekio Ave. 3, LT-10257 Vilnius, Lithuania
[2]Department of Polymer Chemistry and Technology, Kaunas University of Technology, Radvilėnų Rd. 19, LT-50254 Kaunas, Lithuania
domantas.berenis@ff.stud.vu.lt

Organic light-emitting diodes (OLEDs) have attracted significant attention for their ease of fabrication, and high energy efficiency. In recent years, thermally activated delayed fluorescence (TADF) materials have emerged as a promising alternative to currently utilized phosphorescent emitters, achieving 100% internal quantum efficiency without the need for heavy metals [1]. However, developing stable and efficient blue OLEDs presents challenges due to the more energetic nature of the blue light which increases the probability of device degradation through bimolecular processes. Host materials play a vital role in optimizing device performance by facilitating efficient energy transfer and suppressing detrimental intermolecular interactions. Therefore, engineering a proper host material for the emissive layer of blue OLEDs is crucial.

In this work, we investigate 4 novel OLED host materials (fig. 1). Materials contain tert-butyl and CN substituents that aid in inhibiting intermolecular interactions and enhancing electron transfer character, respectively. Additionally, RB134, RB135 contain carbazole electron donor units connected to the main molecule core by the CC bond rather than the weaker C-N bond.

Photophysical, electrochemical studies of novel hots as well as performance of blue OLED devices are presented. Novel hosts exhibit significantly high singlet and triplet excited state energies as well as nanosecond photoluminescence decay times, enabling their successful utilization in OLED fabrication.

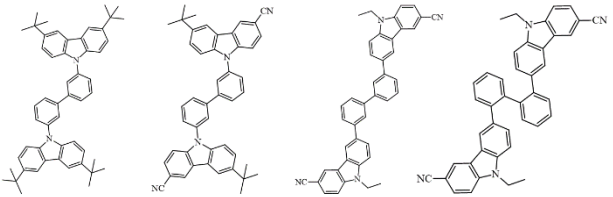

Fig. 1. Molecular structures of studied host materials

Keywords: *OLED, electroluminescence, organic, optoelectronics, TADF.*

References:

1. H. Uoyama et al. *Nature* **492(7428)** p. 234–238 (2012)

P30. Unlocking the Potential of Phenylethenyl-Substituted Phenoxazine and Phenothiazine Derivatives: Aggregation-Induced Emission Enhancement for High-Performance, Non-Doped OLEDs

Ehsan Ullah Rashid[1], Monika Cekaviciute[1], Jurate Simokaitiene[1], Juozas Vidas Grazulevicius[1], Dmytro Volyniuk[1], Khrystyna Ivaniuk[2], Pavlo Stakhira[2]

[1]Department of Polymer Chemistry and Technology, Kaunas University of Technology, K. Barsausko St. 59, 51423 Kaunas, Lithuania
[2]Lviv Polytechnic National University, S. Bandera 12, 79013 Lviv, Ukraine
ehsan.rashid@ktu.edu

This work presents synthesis of phenoxazine, and phenothiazine substituted with phenylethylene using mono-step Buchwald-Hartwig approach for the sake of highly efficient organic light emitting diodes (OLEDs) with blue emission. Absorption of solution of compounds is ca. 310 nm and emission ca. 500 nm which gives cyan blue emission. The dispersion of these compounds in water-THF mixes shows a notable increase in aggregation-induced enhanced emission (AIEE) with increasing water fraction. The photoluminescence quantum yields of the compounds dissolved in toluene range from 3% to 26%, whereas in solid films, they elevate significantly, ranging from 5.25% to 53%. This notable shift is unequivocally linked to the phenomenon of AIEE. We employed density functional theory computational analysis to ascertain critical parameters including optimized molecular geometries, frontier molecular orbitals, intramolecular charge transfer, excitation energies, and corresponding wavelengths. Internal reorganization energy for compounds is calculated using Marcu's theory which demonstrates significant propensity for hole mobility. Thermal analysis revealed the compounds have high melting and decomposition temperature. Based on cyclic voltammetry, the compounds' estimated ionization potentials and electron affinities are 5.13–5.31 eV and 2.08–2.24 eV, respectively. OLEDs incorporating the synthesized compound as the primary emitter exhibit a distinctive bluish-cyan emission, characterized by an electroluminescence intensity peaking at approximately 500 nm. These devices showcase remarkable luminance exceeding 1000 cd/m², coupled with external quantum efficiencies spanning from 2.5% to 6%, marking a significant stride forward in OLED technology.

Keywords: *organic light emitting diode, aggregation induced enhance emission, phenoxazine, phenothiazine, density functional theory, reorganization energy.*

P31. Enhanced coherent optical effects in Ξ-shaped hybrid quantum-plasmonic systems

Hamid Reza Hamedi[1], Julius Ruseckas[1], Vassilios Yannopapas[2], Emmanuel Paspalakis[3]

[1]Baltic Institute of Advanced Technology, Pilies St. 16-8, LT-01403 Vilnius, Lithuania
[2]School of Applied Mathematical and Physical Sciences, Department of Physics, National Technical University of Athens, 157 80 Athens, Greece
[3]Materials Science Department, School of Natural Sciences, University of Patras, 265 04 Patras, Greece
Hamid.r.hamedi@gmail.com

We investigate coherent optical phenomena exhibited by a hybrid quantum plasmonic system composed of four energy levels, featuring two closely spaced uppermost energy levels interacting with a weak probe field and a strong control field (Fig. 1(a)). The lower leg of the system engages with the free-space vacuum, while the upper leg responds to interactions with surface plasmons (fig. 1(b,c)). We reveal a significant transformation in the absorption and dispersion characteristics of this quantum system, influenced by the interplay between quantum interference resulting from the presence of plasmonic nanostructures [1] and the effects of incoherent pumping. In the absence of an incoherent pump field we observe the emergence of multiple distinct absorption profiles, each containing optical transparency windows nestled amidst absorption spectral peaks. Introduction of an incoherent pump field leads to two well-defined symmetrical gain dips, each separated by a frequency corresponding to the dressed eigenstates of the system. This unique gain behaviour persists whether or not population inversion occurs. We also show that these effects can be complemented with the existence of fast or slow light, expanding the range of optical phenomena that can be harnessed within this quantum system [2].

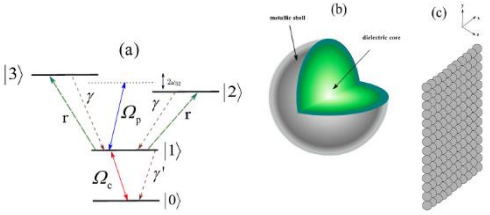

Fig. 1. (a) The level structure of a quantum emitter (QE) in Ξ configuration. A metal-coated dielectric nanosphere (b) and a 2D array of such spheres (c)

Keywords: *hybrid quantum-plasmonic systems, transparency window, gain.*

References:

1. Sofia Evangelou et al. *Phys. Rev. A* **86** p. 053811 (2012)
2. Hamid R. Hamedi et al. *Eur. Phys. J. Plus* **139** p. 314 (2024)

P32. Application of the Modified Salan-type Ligands to the Cu^{2+} and Fe^{3+} Optical Detection in Aqueous Media

Iryna Tepliakova[1], Roman Viter[1], George Kostakis[2], Martin Sahul[3]

[1]Institute of Atomic Physics and Spectroscopy, University of Latvia, Jelgavas St. 3 "House of Science", LV-1004 Riga, Latvia
[2]Department of Chemistry, School of Life Sciences, University of Sussex, Sussex House, Falmer Brighton, BN1 9RH, United Kingdom
[3]Faculty of Materials Science and Technology, University of Technology, J. Bottu St. 25, 917-24 Trnava, Slovak Republic
iryna.tepliakova@lu.lv, roman.viter@lu.lv, g.kostakis@sussex.ac.uk

Ligands with chelating properties, such as Schiff bases, imines, and Salan-type ligands, are promising materials for photochemical sensors of metal ions, which require good sensitivity and selectivity. The ability of such ligands to host metal ions in their molecular structure and specific optical properties, such as high intensity photoluminescence, create new opportunities to define metal ion concentration in aqueous media by optical methods with fairly high accuracy. In addition, the structure of the ligand could be chemically tuned according to the requirements of the sensor [1].

In this work, the sensitivity and selectivity of modified Salan-type ligands were investigated by photoluminescence **(PL)** and transmittance **(TM)** methods.

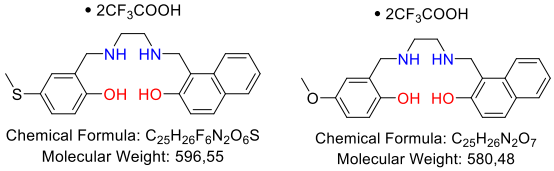

Fig.1 Chemical structure of investigated ligands

Salan ligands were synthesized in salt form to make them soluble in water and alcohols. For sensor testing, the ligands and metal salts were dissolved in ethanol at a concentration of 100 mM/L.

Sensor testing was performed in a home-built system with a quartz cuvette equipped with a magnetic stirrer, Fiber optic spectrometer, system of lenses and filters, Fiber optic cables, and a portable 325 nm UV light source with detector. During the measurement steady-state PL and TM spectra were saved after each metal ion probe. The kinetics of local PL and TM peaks were recorded. The sensitivity to Cu^{2+} and Fe^{3+} ions in sub micromolar range was observed. Complex formation of ligand with Cu and Fe was proofed by FTIR. Mechanisms of interaction were proposed, main sensors parameters were calculated.

Keywords: *photochemical sensors, metal ions detection, chelators.*

References:

1. S. Memon et al. *Curr Anal Chem* **10** p. 393–417 (2014)

P33. Electron-Poor Acridones and Acridiniums as Super Photooxidants in Molecularp Hotoelectrochemistry by Unusual Mechanisms

Jonas Žurauskas[1,2], Paulius Vaickūnas[1], Soňa Boháčová[3], Shangze Wu[2], Valeria Butera[4], Simon Schmid[2], Michał Domański[2], Tomáš Slanina[3], Joshua Philip Barham[2], Edvinas Orentas[1]

[1]Vilnius University, Lithuania
[2]University of Regensburg, Germany
[3]Institute of Organic Chemistry and Biochemistry, Czech Republic
[4]Central European Institute of Technology, Czech Republic
jonas.zurauskas@chemie.uni-regensburg.de

Electron-deficient acridones and in situ generated acridinium salts are reported as potent, closed-shell photooxidants that undergo surprising mechanisms. When bridging acyclic triarylamine catalysts with a carbonyl group (acridones), this completely diverts their behavior away from open-shell, radical cationic, 'beyond diffusion' photocatalysis to closed-shell, neutral, diffusion-controlled photocatalysis. Bronsted acid activation of acridones dramatically increases excited state oxidation power (by +0.8 V). Upon reduction of protonated acridones, they transform to electron-deficient acridinium salts as even more potent photooxidants ($^{*}E_{1/2}$ = +2.56–3.05 V vs SCE). These oxidize even electron deficient arenes where conventional acridinium salt photooxidants have thusfar been limited to electron-rich arenes. Surprisingly, upon photoexcitation these electron-deficient acridinium salts appear to undergo two electron reductive quenching to form acridinide anions, spectroscopically-detected as their protonated forms. This new behaviour is partly enabled by a catalyst preassembly with the arene, and contrasts to conventional SET reductive quenching of acridinium salts. Critically, this study illustrates how redox active chromophoric molecules initially considered photocatalysts can transform during the reaction to catalytically active species with completely different redox and spectroscopic properties [1].

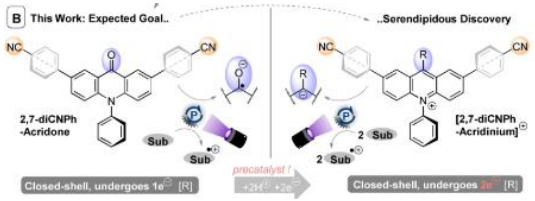

Fig. 1. Acridone and acridinium salt closed-shell super photo-oxidants

Keywords: *electrophotocatalysis, e-PRC, photoredox, catalysis, chromophore, photooxidant.*

References:

1. J. Žurauskas et al. *Angewandte Chemie* **135** p. e202307550 (2023)

P34. Exploration of Novel Monomeric and Hexameric Anthracene Derivatives for Triplet-Triplet Annihilation Upconversion

Justas Lekavičius[1], Paulius Baronas[2], Maciej Majdecki[3], Przemysław Gaweł[3], Kasper Moth Poulsen[2], Karolis Kazlauskas[1]

[1]Institute of Photonics and Nanotechnology, Vilnius University, Saulėtekio Ave. 3, LT-10257 Vilnius, Lithuania
[2]Department of Chemical Engineering, Universitat Politècnica de Catalunya, EEBE, Eduard Maristany 10–14, 08019 Barcelona, Spain
[3]Institute of Organic Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland
justas.lekavicius@ff.vu.lt

Triplet-triplet annihilation mediated photon upconversion (TTA-UC) is a process that increases the energy of incoherent light using triplet-sensitized organic molecules, called the annihilator. Potential applications of TTA-UC span across various fields, including targeted drug delivery, photocatalysis, and photovoltaics [1]. In solar cells, the UC process could serve as a tool to overcome the Shockley-Queisser limit by harvesting sub-bandgap photons. However, there are numerous factors limiting the UC quantum yield (ϕ_{UC}), such as annihilator aggregation and low probability of singlet state generation through TTA. Therefore, it is essential to search for novel annihilators that could overcome these obstacles.

In this work two novel anthracene derivatives (Anc-mono and Anc-hex) were paired with porphyrin-based PdTPBP and PtTPBP triplet sensitizers (see fig. 1). Anc-mono and Anc-hex annihilators have similar fluorescence quantum yields of 95.5% and 84.0% respectively. However, concentration screening of all four sensitizer:annihilator UC solutions show that PtTPBP:Anc-mono UC system has the highest ϕ_{UC}, which is close to 20%, whereas UC solutions with Anc-hex display 10-fold lower ϕ_{UC} values. Various spectroscopy measurements were performed to provide a fundamental explanation for this tendency and other results.

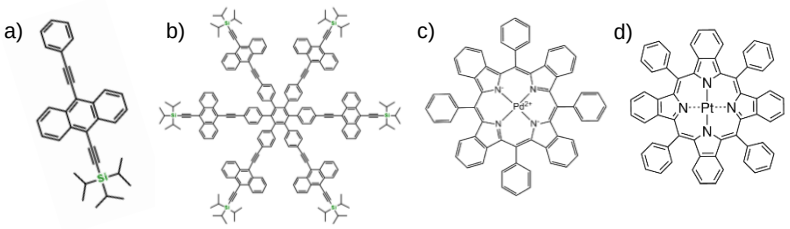

Fig. 1. Chemical structures of molecules: a) Anc-mono b) Anc-hex c) PdTPBP d) PtTPBP

Keywords: *photon upconversion (UC), triplet-triplet annihilation (TTA), organic light emitters.*

References:

1. L. Zeng et al. *Acc. Chem. Res.* **55** p. 2604–2615 (2022)

P35. Photophysical Study of Purine-based Metal Ion Sensors

Kamilė Tulaitė[1], Justina Jovaišaitė[1], Irina Novosjolova[2], Maris Turks[2], Gediminas Jonušauskas[3], Saulius Juršėnas[1]

[1]Institute of Photonics and Nanotechnology, Vilnius University, Sauletekis Ave. 3, LT-10222 Vilnius, Lithuania
[2]Institute of Technology of Organic Chemistry, Riga Technical University, Valdena St. 3, LV-1048 Riga, Latvia
[3]Laboratoire Ondes et Matière d'Aquitaine, Bordeaux University, UMR CNRS 5798, 351 Cours de la Liberation, 33405 Talence, France
kamile.tulaite@ff.vu.lt

The purine heterocyclic system plays a crucial role in biological and medicinal chemistry due to its involvement in genetic information transcription and translation. Despite extensive efforts to enhance purine functionalities, there is a need for novel, biocompatible materials derived from the purine core. These materials show potential as chemical sensors, fluorescence imaging agents, photocatalysts, and photodynamic therapy (PDT) sensitizers activated by light, including solar illumination.

The purine core is advantageous for chemical modification because of well-established synthetic methods and its structure, featuring five attachment points for substitutions. Electron-donating groups can be added at the C2, C6, or C8 positions. Expanding the functionality of purine derivatives can be achieved through long-lived excited triplet or radical states, and by shifting steady-state absorption towards the visible or near-infrared range. These modified purine derivatives have proven effective as emitters in OLEDs, pH sensors, and imaging tools for cell compartments [1]. Recently, purines have also been reported as effective metal ion sensors, particularly derivatives with an external C8-complexing arm working with the purine N7. However, examples leveraging both the C6-substituent and the purine N7 are limited.

This study presents a detailed photophysical analysis of purine-based derivatives' complexation processes in polar solvents and aqueous media for chemical sensors. Various characterization techniques, including steady-state absorption, fluorescence, and time-resolved fluorescence spectroscopy, were employed. Several sensor prototypes were demonstrated for detecting metal ions such as alkali, alkaline earth, heavy, and transition metals, applicable in industry (using acetonitrile) and biology/environment (using water). The synthesized compounds detected traces of transition and heavy metal ions at ppb levels. New water-soluble compounds ZiK-740 and ZiK-772 exhibited high sensitivity to mercury (II) ions in water.

Keywords: *purine, metal ion sensor, fluorescence sensor.*

References:

1. J. Jovaisaite et al. *Phys. Chem. Chem. Phys.* **22(45)** p. 26502–26508 (2020)

P36. Photothermal Activity of Silver Nanoparticles for Polymer Shape Memory Activation

Katrina Krizmane, Virginija Vitola, Milena Dile, Aleksejs Zolotarjovs

Institute of Solid State Physics, University of Latvia, Kengaraga St. 8, LV-1063 Riga, Latvia
katrina.krizmane@cfi.lu.lv

Silver nanoparticles, within the size range from 10 to 40 nm exhibit ideal photothermal characteristics [1]. These nanoparticles can absorb light and convert that into heat. When incorporated into a polymer matrix, they can significantly improve the polymer's shape-memory characteristics. Typically, a polymer must be heated above its glass transition temperature to return to its original shape. However, the integration of silver nanoparticles enables this transformation through light exposure alone, eliminating the need for conventional heating methods. This advancement holds promising implications for medical applications, particularly in the treatment of vascular diseases, where localized and controlled heating can induce shape recovery without invasive procedures [2].

This research investigates the temperature dependence of silver (Ag) nanoparticles synthesized using polyvinylpyrrolidone (PVP) of varying molar masses. The nanoparticles were prepared via a microwave-assisted polyol method, and their morphology was characterized through scanning electron microscopy (SEM).

Acknowledgements: The financial support provided by Scientic Research LZP FLPP No. lzp-2023/1-0521 Light Activated 4D Printed Materials for Vascular Tissue Engineering is greatly acknowledged.

Keywords: *silver nanoparticles, photothermal effect.*

References:

1. L. A. Austin et al. *Arch Toxicol* **88** p. 1391–1417 (2014)
2. V. Vitola et al. *J Polym Res* **28** p. 13 (2021)

P37. Donor-π-Acceptor (D-π-A) Based Solid State Emitters for Organic Light Emitting Diodes (OLEDs)

Khushdeep Kaur, Asta Dabuliene, Juozas Vidas Grazulevicius

Department of Polymer Chemistry and Technology, Kaunas University of Technology, K. Barsausko St. 59, 51423 Kaunas, Lithuania
khushdeep.kaur@ktu.edu

D-π-A based solid state emitters are promising candidates for OLEDs, fluorescence imaging devices, solid-state lasers, chemical sensors etc., owing to their ease of fabrication and tunable structures [1]. Non-linear optical (NLO) activity is also considered as a fundamental property to check device performance [2]. The rising demand of single layer devices over multilayer devices make it essential to design and synthesize emissive materials capable of transporting both holes and electrons [3]. Furthermore, charge transport properties and optical properties (linear and non-linear) of semiconducting devices are greatly influenced by nature of donor, π-bridge and acceptor fragments [2,3]. In a recent report, NLO susceptibility of (E)-2-(3-(4-bromostyryl)-5,5-dimethylcyclohex-2-en-1-ylidene)malononitrile was reported to be higher than that of the previously reported compounds [4]. With the aim to develop novel bipolar semiconducting materials, a series of new D–A materials were designed and synthesized by selecting (E)-2-(3-styryl-5,5-dimethylcyclohex-2-en-1-ylidene)malononitrile as an acceptor and carbazole, thianthrene, phenoxathiine or fluorene fragments as a donor fragment coupled via π bridge. In order to establish the structure-property relationship, we systematically studied their photophysical, thermal, and electroluminescent properties. Thus, the newly synthesized D-A materials could be suitable for photonic and optical devices particularly for organic photodetectors.

Keywords: *D-π-A, solid-state emitters, OLEDs, carbazole, fluorene, dithianthrene, phenoxathiine etc.*

References:

1. Zheng Zheng et al. *J. Org. Chem.* **78(7)** p. 3222–3234 (2013)
2. Shivani et al. *J. Phys. Chem. C.* **127(2)** p. 1260–1272 (2023)
3. Tao Lin et al. *Chem Phy* **440** p. 47–52 (2014)
4. D. Bharath et al. *Opt. Laser Technol.* **59** p. 24–31 (2014)

P38. Optical Characterization of Au Nanoparticle-TiO_2 Heterostructures Employing Experimental and Computational Methods

Klaudijus Midveris[1], Tomas Klinavičius[1], Domantas Peckus[1,2], Andrius Vasiliauskas[1], Šarūnas Meškinis[1], Asta Tamulevičienė[1,2], Tomas Tamulevičius[1,2]

[1]Institute of Materials Science, Kaunas University of Technology, K. Baršausko St. 59, LT-51423 Kaunas, Lithuania
[2]Department of Physics, Kaunas University of Technology, Lithuania
klaudijus.midveris@ktu.lt

There is a great interest in heterostructure photocatalysts comprised of semiconductors, coupled with Au nanoparticles due to their importance in the efficient water-splitting processes under solar illumination. The use of computational techniques, such as the transfer matrix method and experimental methods, such as spectroscopic ellipsometry and transient absorption spectroscopy, allows spectral response characterization of such heterostructures [1–3]. This work investigates the effective medium morphology of Au/TiO_2 heterostructures and its influence on the spectral extinction, optical constants and electron-phonon interactions of the aforementioned material assemblies.

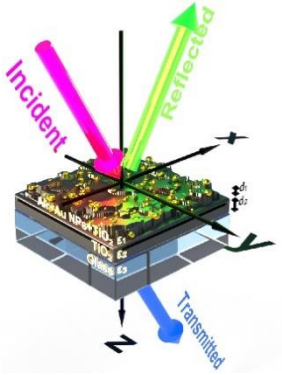

Fig. 1. Conceptual illustration of the Au/TiO_2 heterojunction spatial arrangement

Acknowledgements: The work was supported by the Research Council of Lithuania (LMT) project No. S-MIP-23-93.

Keywords: *Au/TiO_2 heterostructures, ellipsometry, transfer matrix method, transient absorption spectroscopy.*

References:

1. R. Raymond et al. *Progress in Electromagnetics Research B*. **35** p. 241–261 (2011)
2. M. Horprathum et al. *Journal of Physics: Conference Series* **417** p. 012007 (2013)
3. Luchao Du et al. *Journal of Applied Physics* **128** p. 213104 (2020)

P39. Optimizing ZnS:Cu-Based Electroluminescent Films for Flexible Optoelectronic Applications

Madara Klave, Milena Dile, Marija Dunce, Ernests Einbergs, Aleksejs Zolotarjovs

Institute of Solid State Physics, University of Latvia, Riga, Kengaraga St. 8, LV-1063, Latvia
madara.klave@cfi.lu.lv

Electroluminescent materials play a critical role in the development of advanced optoelectronic devices. Among these materials, ZnS:Cu is a well-known phosphor with potential applications in flexible displays and lighting systems. The study investigates ZnS:Cu embedded in polyurethane thick films deposited by tape-casting method on Fluorine Tin Oxide (FTO)-coated glass substrate with a colloidal graphene top electrode. When applying alternating current (AC), electroluminescence was observed. The influence of film thickness, ZnS:Cu/polyurethane concentration, applied AC voltage and frequency on electroluminescent performance was explored. Our findings indicate that optimizing these parameters can significantly enhance the performance of AC powder electroluminescence (ACPEL) devices.

The work contributes to the design of flexible, efficient electroluminescent materials, paving the way for their practical implementation in next-generation optoelectronic applications.

Keywords: *electroluminescence, ACPEL, ZnS:Cu.*

P40. Improving the Statistical Factor of Perylene via TIPS Functionalization

Manvydas Dapkevičius[1], Steponas Raišys[1], Lukas Naimovičius[1,2], Kasper Moth-Poulsen[2], Karolis Kazlauskas[1]

[1]Institute of Photonics and Nanotechnology, Vilnius University, Universiteto St. 3, LT-01513 Vilnius, Lithuania
[2]Department of Chemical Engineering, Universitat Politècnica de Catalunya, EEBE, Eduard Maristany 10–14, 08019 Barcelona, Spain
manvydas.dapkevicius@ff.stud.vu.lt

Photon upconversion (UC) can be achieved through triplet fusion when two lower energy triplet excitons are combined to create one, larger energy singlet exciton. This phenomena has potential in increasing solar cell efficiency, targeting drug delivery *in vivo* and many other applications [1]. UC system consists of two molecules: sensitizer, which absorbs lower energy light and converts the formed singlet to a triplet state, and an annihilator, which fuses triplet excitons into a emissive singlets. UC is a multi-step process where triplet fusion yield is considered the limiting one. Statistical factor describes annihilator's efficiency of triplet fusion into singlet states. Recently it was reported that Perylene has a statistical factor of 17.9% [2], which, in this work, was improved more than 2-fold by the addition of TIPS moieties (fig. 1).

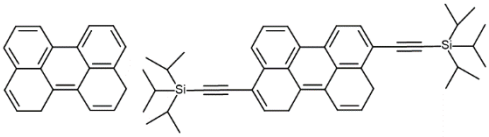

Fig. 1. Perylene and TIPS functionalized counterpart

A comprehensive photophysical analysis of the UC system with TIPS-functionalized perylene demonstrated increased statistical factor up to 41.1%. This was attributed to a change in spin direction at the triple bond suggesting the presence of a singlet-like character for triplet species, leading to enhanced coupling between triplet-triplet pair with the first singlet state. Higher statistical factor allowed to achieve UC quantum yield of 13.7% which is a record high value in the emission range of 470–540 nm.

Keywords: *upconversion, perylene, triplet-triplet annihilation, triplet fusion.*

References:
1. J. Zhou et al. *Chemical Reviews* **115(1)** p. 395–465 (2014)
2. L. Naimovičius et al. *Journal of Materials Chemistry C* **11(42)** p. 14826–14832 (2023)

P41. Donor-Ornamented Derivatives of Benzodioxinoquinoxaline Enabling Solid-State-Enhanced RTP/TADF and High Charge Carrier Mobilities

Mariia Stanitska[1], Lilia Deva[2], Levani Schirtladze[3], Glib Baryshnikov[3], Dmytro Volyniuk[1], Pavlo Stakhira[2], Juozas Vidas Gražulevicius[1]

[1]Kaunas University of Technology, Baršausko St. 59, 51423 Kaunas, Lithuania
[2]Lviv Polytechnic National University, Stepan Bandera St. 12, 79013 Lviv, Ukraine
[3]Linköping University, Norrköping, SE-60174, Sweden
mariia.stanitska@ktu.edu

Quinoxaline-derived compounds are among the mostly used emitters in fabrication of efficient yellow, orange and red organic light-emitting diodes (OLEDs) since they are characterized by inherently low optical band gap as well as high thermal and electrochemical stability [1,2]. In the context of structural design, the D-A-D architecture, where electron donors are situated in *ortho*-position to quinoxaline acceptor, is beneficial as it imposes highly twisted molecular conformation that restricts rotational freedom of donor fragments and results in higher photoluminescence quantum yield (PLQY) of the compounds. To address the usually low charge carrier mobilities of highly twisted donor-acceptor-type compounds that exhibit thermally activated delayed fluorescence (TADF), we designed a rod-like acceptor known as benzodioxinoquinoxaline. This acceptor and two derivatives were synthesized *via* microwave Buchwald-Hartwig cross-coupling reactions with yields of up to 91%, using acridine or phenoxazine. The compounds exhibited three different types of photoluminescence, that is well supported by quantum chemical calculations. Benzodioxinoquinoxaline showed blue fluorescence, with a very short lifetime of 0.64 nanoseconds. Others exhibited either green solid-state-enhanced TADF (SSE-TADF) or room temperature phosphorescence (RTP) with lifetimes of approximately 6–7 milliseconds. In a polymeric host, the samples achieved photoluminescence quantum yield of close to 30%. The derivatives containing acridine or phenoxazine exhibited bipolar charge transport. At an electric field of 5.8×10^5 V/cm, hole and electron mobilities respectively reached $3.2\cdot10^{-4}$ and $1.5\cdot10^{-4}$ $cm^2V^{-1}s^{-1}$ for the phenoxazine-based compound. Among the studied SSE-TADF organic light-emitting diodes, this compound demonstrated the highest external quantum efficiency of 12.3% due to its good charge-transporting and SSE-TADF parameters.

Keywords: *microwave irradiation-assisted Buchwald-Hartwig cross-coupling reaction, benzodioxinoquinoxaline, acridan, phenoxazine, solid-state-enhanced thermally activated delayed fluorescence, room temperature phosphorescence, organic light-emitting diode.*

References:

1. P. Ledwon et al. *Dye. Pigment.* **173** p. 108008 (2020)
2. Z. Wen et al. *J. Mater. Chem. C* **10** p. 3396–3403 (2022)

P42. Application of Recycled PVB as Encapsulant for PV Modules

Matas Rudzikas[1,2], Egle Fataraitė Urbonienė[1,3], Beatriz Yécora[4], Tamara Oroz[4], Filip Brkić[5]

[1]"The Applied Research Institute for Prospective Technologies", Vismaliuku St. 34, LT-10243 Vilnius, Lithuania;
[2]JSC "Modern E-Technologies", Vismaliuku St. 34, LT-10243 Vilnius, Lithuania;
[3]Kaunas University of Technology, K. Donelaičio St. 73, LT-44029 Kaunas, Lithuania
[4]Lurederra", Industrial Area Perguita, C/A Nº 1 31210, Los Arcos, Navarra, Spain
[5]BIO-MI, Put Brdo 15, 51 211 Matulji, Croatia
matas.rudzikas@protechnology.lt

The capacity of photovoltaic (PV) installations annually increases and end-of-life PV panels waste by 2050 could reach 60–78 Mt [1]. While materials like glass, silicon, and metals (Ag, Pb, Cu, Sn) commonly found in PV panels are recyclable [2], the usual encapsulant material, ethylene vinyl acetate (EVA), presents recycling challenges. To overcome this, polyvinyl butyral (PVB) emerges as a viable alternative due to its recyclability.

The investigation aimed to validate the feasibility of using primary and recycled PVB film with standard PV module production equipment.

Commercial EVA and PVB, as well as recycled PVB obtained from automotive glass waste via a specialized mechanochemical process developed by Lurederra Technological Centre, was utilized in this study. Glass samples (10x10 cm) were laminated with both commercial and recycled encapsulants, in a flat-bed laminator, with some samples also employing butyl edge sealant for edge isolation. Subsequently, samples were exposed to a damp heat test (IEC 61215) in a climatic chamber.

The lamination process resulted in successful samples without defects such as bubbles or delaminations. After 250 hours in the climatic chamber, no discernible changes were observed. However, after 500 hours, samples absent of edge sealant exhibited fogging, particularly around the edges, indicative of moisture penetration. The changes in adhesion between layers was also evaluated before and after damp heat tests.

Comparative analysis revealed minor differences in average transmittance among the laminated samples: for commercial PVB and EVA it was respectively 70.24% and 68.71%, and for recycled PVB it was 68.37%.

Acknowlegments: The work was supported by the project SUNRISE, which received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 958243.

Keywords: *photovoltaic module, encapsulant, polyvinyl butyral, recycling.*

References:

1. S. Weckend et al. (2016)
2. A. Divya et al. *Solar Energy Materials and Solar Cells* 253 (Elsevier B.V., 2023)

P43. Harnessing Twisted Phenothiazine and Phenothiazine Sulfone Derivatives as Emitters and HTMs for Efficient Doping Free Fluorescent and Multiple-Resonance TADF OLEDs

Melika Ghasemi[1], Ramakant Gavale[2], Faizal Khan[2], Dmytro Volyniuk[1], Juozas Vidas Gražulevičius[1], Rajneesh Misra[2]

[1]Department of Polymer Chemistry and Technology, Kaunas University of Technology, K. Baršausko St. 59, LT-51423 Kaunas, Lithuania
[2]Department of Chemistry, Indian Institute of Technology Indore, Khandwa Rd., Simrol, Madhya Pradesh 453552, India
melika.ghasemi@ktu.edu

Spin statistics dictate that upon electronic excitation, singlet and triplet excitons are generated in a 1:3 ratio. However, only singlet excitons contribute to photon emission, utilizing 25% of the exciton generation factor, resulting in an external quantum efficiency (EQE) of 5–7.5% in devices [1,2]. The efficiency and stability of organic light-emitting diodes (OLEDs) rely on factors like photoluminescence quantum yield (PLQY) and charge transportation and recombination. Twisted organic compounds play a significant role in the development of solid-state fluorescent materials and have gained substantial attention owing to their potential applications in optoelectronic devices [3].

A series of metal-free twisted organic compounds integrating phenothiazine and phenothiazine sulfone moieties were designed, synthesized, and characterized to ascertain their viability as blue/green emitters as well as hole transporting layers (HTLs) within OLEDs. The study delved into discerning the impact on the efficiencies of the devices based on the presence and absence of donor moiety. The photophysical studies unveiled that all the compounds exhibit fluorescence, PLQYs of up to 39.64%, good thermal stability and hight hole transporting capabilities (1.56×10^{-4} cm^2/Vs and 1.27×10^{-4} cm^2/Vs at 5×10^5 V/cm electric field), thus rendering them suitable for OLED applications. The compounds were implemented as emissive layers within doping-free fluorescent devices, and as HTLs in multiple-resonance thermally activated OLEDs, achieving an EQE of 4.33%, 7.45% and turn on voltage of 3.60V, 4.60V, respectively.

Acknowledgements: This work was supported by funding from the Research Council of Lithuania (Project “ELOS” No S-MIP-21-7).

Keywords: *organic light-emitting diodes, fluorescence, hole transporting, phenothiazine, phenothiazine sulfone, tetraphenylethylene.*

References:

1. H. Kaji et al. *Nat. Commun.* **6** p. 1–8 (2015)
2. J. Wang et al. *Journal of Photochemistry and Photobiology C: Photochemistry Reviews* **17** p. 69–104 (2013)
3. P. S. Hariharan et al. *Dyes and Pigments* **174** p. 108067 (2020)

P44. Quinoxaline-Based Derivatives as Red Emission Organic Luminophores, Synthesis and Investigation

Mohamed Hassan Saad Abdella, Matas Guzauskas , Jurate Simokaitiene, Juozas Vidas Grazulevicius

Department of Polymer Chemistry and Technology, Kaunas University of Technology, K. Barsausko St. 59, LT-51423 Kaunas, Lithuania
mohamed.abdella@ktu.edu

As next-generation materials for optoelectronic devices, organic luminescent materials with triplet exciton harvesting capabilities are beneficial [1]. Because of their inexpensive cost, flexible and environmentally friendly synthesis, superior stability, and room temperature phosphorescence (RTP) or thermally activated delayed fluorescence (TADF) properties, organic luminophores are an attractive alternative to organic metal complexes [2].

In this work, a series of quinoxaline-based compounds as building blocks for the development of red TADF or RTP materials were synthesized. The quinoxaline moiety's prolonged conjugation length and electron acceptor properties allow diphenyl- and a-based compounds have RTP characteristics, according to photophysical examination. Compared to quinoxaline derivatives without bromine, quinoxaline compounds containing a bromine moiety exhibited more effective RTP. Because of the heavy atom effect, the addition of bromine atoms improved the RTP characteristics [2]. Phenothiazine-containing compounds showed red TADF with short emission lifetimes.

Keywords: *room temperature ph*osphores*cence, quinoxaline, brominated compounds, phenothiazine.*

References:

1. Przemyslaw Data et al. *Chem. Asian J.* **14** p. 1613 – 1636 (2019)
2. Z. Xu et al. *Mater. Adv.* **2** p. 5777 (2021)
3. M. Ghaemy et al. *Polym. Sci.* **124** p. 1707 (2012)
4. L. Skhirtladze et al. *Materials (Basel)* **16** p. 1294 (2023)

P45. Plasmonic Diffraction Gratings for THz Emission

Mohammad Esmaeil Daraei, Ignas Nevinskas

Center for Physical Sciences and Technology, Department of Optoelectronics
Saulėtekio Ave. 3, LT-10257 Vilnius, Lithuania
esmaeil.daraei@ftmc.lt

Terahertz (THz) frequencies refer to the region between the millimeter wave and infrared bands in the electromagnetic (EM) spectrum, typically between 0.1 to 10 THz [1]. Many potential applications have been identified which include imaging, defence, security, biology and medicine. Among various techniques for THz generation, photoconductive antennas (PCAs) have been extensively utilized to generate pulsed terahertz radiation. In recent studies, plasmonic nanostructures have been utilized to increase the THZ PCA efficiency. The plasmonic nanostructures interact with the input laser light and enhance optical absorption in the active photoconductive region resulting in higher free carrier concentration and carrier gradients.

In our research, we have used Finite-Difference Time-Domain (FDTD) modeling. Our structure consists of a semiconductor crystal. On top of this crystal a fabricated gold nanostructure interacting with a laser pulse would induce the surface plasmons. The plasmons would be absorbed by the semiconductor in a significantly smaller volume than that dictated by the absorption depth. The generated gradient of photoexcited charge carriers would induce ultrafast photocurrents, which in turn would emit a THz pulse. The optimized dimensions of gold grating found 320 nm width and 120 nm height. The schematic of our structure and absorption gradient induced by SPPs have been shown in fig.1. Our simulations show that the absorption rate is about 33 percent without plasmonic grating, while adding a plasmonic grating will result in 45 percent absorption and this will finally lead to a higher and sharper THz pulse radiation.

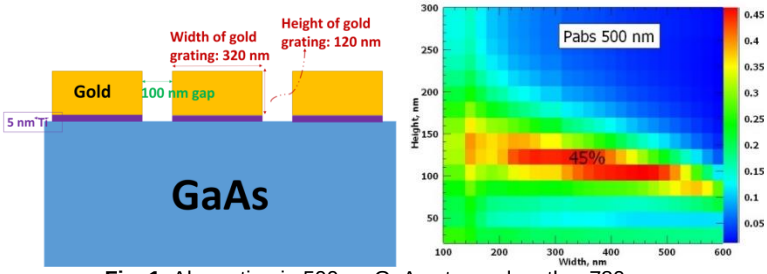

Fig. 1. Absorption in 500nm GaAs at wavelength = 780 nm

Keywords: *Terahertz (THz) emission, Photoconductive antennas (PCAs), Plasmonic nanostructures, Finite-Difference Time-Domain (FDTD) simulation.*

References:

1. Y. Huang et al. *2011 International Workshop on Antenna Technology (iWAT)* p. 152–156 (2011)

P46. Azimuthal Dependence of Electromagnetically Induced Grating in a Double V-type Atomic System near Plasmonic Nanostructure

Teodora Kirova[1], Seyyed Hossein Asadpour[2], Hamid Reza Hamedi[3], Vassilios Yannopapas[4], Emmanuel Paspalakis[5]

[1]Institute of Atomic Physics and Spectroscopy, University of Latvia, Jelgavas Street 3, Riga, LV-1004, Latvia
[2] School of Physics, Institute for Research in Fundamental Sciences, Lavasani Street 70, Tehran, P.O. Box 19395-5531, Iran
[3]Institute of Theoretical Physics and Astronomy, Vilnius University, Saulėtekio Ave. 3, LT-10257 Vilnius, Lithuania
[4]Department of Physics, National Technical University of Athens, Zografou Street 80, Athens, GR 157 Greece
[5]Materials Science Department, University of Patras, Patras, 26504 Greece
teo@lu.lv

We investigated the performance of Electromagnetically Induced Grating [1] in a four-level atomic system near a plasmonic nanostructure. The plasmonic nanostructure consists of metal-coated dielectric nano-spheres in a periodic 2D arrangement. The double V-type quantum system is coupled by a weak probe laser, a spatially-dependent standing wave, as well as an optical vortex field.

Numerical simulations [2] show that by varying the distance between the plasmonic nanostructure and the quantum system, the amplitude and phase modulations of the transmission function can be modified when the winding number of the vortex light is also altered. When the quantum system is placed close to the plasmonic nanostructure, by adjusting the winding number of the vortex light most of the probe field energy is transferred to the high order, while at larger distances most of this energy is converging in the zero order.

Our work demonstrates a simple scheme for double control over the diffraction efficiency of the 2D grating by using both the winding number of the vortex field and the distance between the plasmonic nanostructure and the quantum system as control knobs. The proposed scheme is advantageous by providing easily achievable manipulation of the grating performance, while it can be realized in typical quantum optics experimental settings, involving hyperfine sublevels of D-lines in alkali-metal atoms.

Keywords: *quantum interference, electromagnetically induced grating, plasmonic nanostructure, optical vortex.*

References:

1. H.-Y. Ling et al. *Phys. Rev. A* **57(2)** p.1338–1344 (1998)
2. S. H. Asadpour et al. *The European Physical Journal Plus* **138** Article number: 246 (2023)

P47. Deep Learning Methods for Colloidal Silver Nanoparticle Concentration and Size Distribution Determination from UV–Vis Extinction Spectra

Tomas Klinavičius[1], Nadzeya Khinevich[1], Asta Tamulevičienė[1,2], Loic Vidal[3], Sigitas Tamulevičius[1,2], Tomas Tamulevičius[1,2]

[1]Institute of Materials Science of Kaunas University of Technology, K. Baršausko St. 59, LT-51423 Kaunas, Lithuania
[2]Department of Physics, Kaunas University of Technology, Studentų St. 50, LT-51368 Kaunas, Lithuania
[3]Institut de Science des Matériaux de Mulhouse IS2M UMR 7361, 15 rue Jean Starcky, F 68100 Mulhouse, France
tomas.klinavicius@ktu.lt

Rapid characterization of colloidal metal nanoparticles (NPs) is of increasing interest for both research and the industry. While direct imaging techniques such as electron microscopy are reliable, they are also expensive, slow and inefficient. On the other hand, an indirect optical tool such as UV-Vis spectroscopy in combination with spectra interpretation related to Mie scattering theory is fast, widely accessible and inexpensive. We present a tandem deep neural network (DNN) for size distribution and concentration prediction of spherical silver (Ag) colloidal nanoparticles synthesized using the seeded growth method. During testing, the tandem DNN provided accurate predictions of NP size distribution characteristics up to 150 nm in radius, with the root mean square percentage error of mean size down to 1.2% [1].

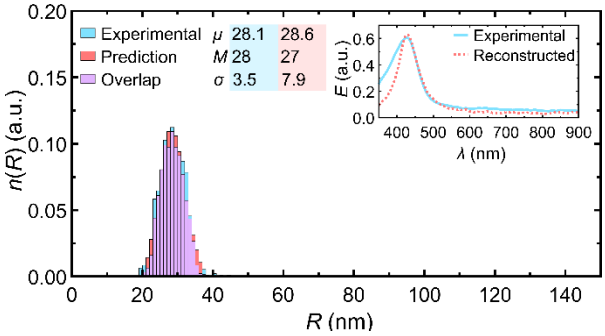

Fig. 1. Example of DNN performance for prediction of size distribution of spherical Ag NPs

Keywords: *nanoparticles, plasmonics, silver, size distribution, deep neural networks, effective medium theory, Mie theory.*

References:

1. T. Klinavičius et al. *The Journal of Physical Chemistry C* **128(23)** p. 9662–9675 (2024)

CERAMICS

P48 – P51

P48. Development of Mullite Based Ceramics using Amorphous Silica from Rice Husk Ash as Alternative Source of Silica

Oji Babatunde, Emmanuel Imoru

Department of Glass and Ceramics, Federal Polytechnic Ado-Ekiti P.M.B 5351, Ekiti State, Nigeria
ojibabatunde2@gmail.com

This research examines the preparation of mullite based ceramics using amorphous silica recycled from rice husk ash (RHA) as alternative source of silica by microwave sintering. The aim is to reduce environmental pollution and convert waste to wealth for industrial application. The recycled waste was characterized to determine Phases, morphology and elemental composition present using, XRD, X-ray fluorescence (XRF) and scanning electron microscope (SEM). The mullite based ceramics were produced by varying percentage composition of the materials and sintering at 1200°C for 3 hours. The developed samples were characterize using XRD,SEM, FTIR, hardness and compression test while physical test like porosity and bulk density were also conducted. The XRF result of amorphous silica from RHA shows 91.325% of SiO_2 while Al_2O_3, CaO, K_20 has 2.447%, 1.845% and 1.547% respectively. The XRD results of developed samples shows increase in mullite phases as percentage composition of amorphous silica increased while FTIR results reveals enhanced bond formation that denotes cohesion of amorphous silica with other constituent materials. The porosity and density test shows that % porosity of samples reduces with increase in amorphous silica while the entire sample shows a reduction in porosity level when compared to the control sample. The samples also showed lower density than the control samples with the highest density value. The SEM images also revealed a uniform particle distribution of materials with the microstructure.

Keywords*: rice husk ash, mullite phase, microwave sintering, amorphous silica, ceramics.*

P49. In-Vitro Bioactivity of Bioceramics Developed by Solid State Sintering using Waste Glass Doped with ZnO Particles

Oji Babatunde, Emmanuel Imoru

Department of Glass and Ceramics, Federal Polytechnic Ado-Ekiti P.M.B 5351, Ekiti State, Nigeria
ojibabatunde2@gmail.com

This research examines the bioactivity of bioceramics material developed using waste glass doped with zinc oxide particles. Waste glass is an industrial and non biodegradable material rich in silica, calcium and oxygen. They constitute environmental menace when sent to landfill however when recycled they can serve as bioactive materials for biomedical application. The bioceramic materials were synthesized via solid state reaction at a temperature of 1100^{o}C with primary phases consisting of combeite and wollastonite as observed after the initial XRD and SEM/EDX analysis after sintering. The samples were prepared using different weight fraction of waste glass and ZnO particles added in percentage ratios of 0:1:2:3 and 4. The samples for in-vitro bioactivity analysis were prepared by soaking the developed samples in a simulated body fluids solution at temperature of 36.5°C for one to seven days before characterization using XRD, SEM/EDX and FTIR analysis. The XRD results shows increasing peaks of hydroxylapatite phase as soaking time increased while the SEM/EDX result indicated a dispersed agglomeration of hydroxylapatite phase on the developed sample surface. The FTIR also showed an increased peak of phosphate ions as apatite layers formed on developed samples. The hardness and compression value showed that samples B and C having 5% and 10% ZnO particles had the best results as compared to the control sample. In the overall five samples of different compositions were examined during the test analysis.

Keywords: *combeite, wollastonite, quartz, bioceramics, hydroxylapatite.*

P50. Porous Mullite Ceramics Modified with Microsized ZrO_2 and WO_3

Ludmila Mahnicka-Goremikina[1], Ruta Svinka[1], Visvaldis Svinka[1], Vadims Goremikins[2]

[1]Institute of Materials and Surface Engineering, Faculty of Natural Sciences and Technology, Riga Technical University, Paula Valdena 3, LV-1048 Riga, Latvia
mahnicka@inbox.lv
[2]Institute of Civil Engineering, Faculty of Civil and Mechanical Engineering, Riga Technical University, Ķīpsalas 6B, LV-1048 Riga, Latvia
goremikins@inbox.lv

The investigation of the improved mullite ceramics properties is actual in our days [1–3]. The porous mullite ceramics modification with magnesia-stabilized zirconia (2.8 mol% MgO) and yttria-stabilized zirconia (8 mol% Y_2O_3), separately, and in a mixture with WO_3, in 1:1 and 1:2 ratios was analysed. Commercially available α-Al_2O_3 and γ-Al_2O_3, amorphous SiO_2 and kaolin were used as raw materials. The porous mullite ceramics were formed by a slip casting of the raw materials slurry. The addition of an Al paste suspension to the slurry used for the pore formation due to the reaction of Al with water and as result due to the H_2 evolution. The dried samples were sintered at 1600°C with the holding time of 1 h.

The zircon and $Al_2(WO_4)_3$ were detected in several samples compositions after XRD results. The microstructure, porosity and pore size distribution as well as thermal properties such as specific heat capacity, thermal conductivity, thermal diffusivity, linear thermal expansion, thermal shock resistance were investigated.

It was stated that the modification of the porous ceramics with mixture of WO_3 and ZrO_2 increases the porosity of samples about 1.5–2 times in comparison with modification separately with WO_3 and ZrO_2. Thus, the high porosity of modified ceramic is about 63–73±2%. The sintered ceramics with a MSZ:WO_3 mixture in a 1:1 ratio with a highest porosity of 73% have the lowest thermal conductivity, lower thermal diffusivity and relatively low specific heat capacity. In turn the mullite ceramics modified with a mixture of MSZ:WO_3 in a 1:2 ratio together with the thermal insulating ability show the best thermal shock resistance during 10 cycles of thermal shock of the scheme 20°C → 1000°C → 20°C with an exposure for 1 h at 1000°C.

Keywords: *mullite ceramics, porous ceramics, WO_3, ZrO_2, thermal properties.*

References:

1. R. Salomão et al. *Interceram Int. Ceram. Rev.* **71** p. 38–50 (2022)
2. M. L. Bouchetou et al. *Ceram. Int.* **45** p. 12832–12844 (2019)
3. L. Gong et al. *J. Porous Mater.* **21** p. 15–21 (2014)

P51. Influence of Zn^{2+} Ions on the Crystallization of Calcium Phosphates under Hydrothermal Conditions

Monika Tiskute, Kestutis Baltakys, Tadas Dambrauskas

Department of Silicate Technology, Kaunas University of Technology, Radvilenų Rd. 19, LT–50270 Kaunas, Lithuania
monika.tiskute@ktu.edu

Calcium phosphates with a molar C/P ratio of 1.61–1.71 naturally occur in human bone, making hydroxyapatite and fluorapatite (Ca/P – 1.67) highly valuable in medical application [1,2]. Synthetic calcium phosphates are biocompatible and widely used in tissue and bone engineering, toothpaste production, implants, and pharmaceuticals. It should be noted that pure hydroxyapatite does not have good antimicrobial properties. In order to improve these characteristics and ensure sterility, calcium phosphate compounds are often modified with various bacteriostatic ions, such as Zn^{2+} ions [3,4]. The aim of this work was to determine the influence of zinc ions on the crystallization of calcium phosphates under hydrothermal conditions.

In the preparation of the initial mixtures, 4 g of calcium carbonate and 0,29 g (1 mol) Zn(NO3)2·6H2O was weighed and transferred into 45 ml PTFE vessels, then mixed with 40 ml of phosphoric acid and distilled water solution. The ratio of calcium and phosphorus was maintained at 1.67. The synthesis was carried out without stirring the suspension in the "Parr instruments" autoclave, at saturated water vapor temperature of 140°C. The isothermal curing durations ware 0 h, 2 h, and 8 h, while the target temperature was reached within 2 h.

At the beginning of synthesis, in the pure CaCO3-H3PO4-H2O system, intensive interaction between the raw materials proceeded, leading to the formation of monetite and hydroxyapatite. Extending the synthesis duration negatively affected the stability of monetite because the intensity of the main diffraction peak (*d* – 0.336 nm) decreased by 2.5 times after 2 h of synthesis and 3.6 times after 8 h of synthesis. The decrease in the intensity of the diffraction peaks characteristic of monetite is related to its recrystallization into hydroxyapatite. When zinc nitrate was added into initial suspension, Zn^{2+} ions was observed to intercalate into the structure of the synthesis products and/or form new compounds. These findings were confirmed by X-ray diffraction (XRD), simultaneous thermal analysis (STA), and Fourier-transform infrared spectroscopy (FT–IR).

Keywords: *monetite, hydroxyapatite, calcium phosphate.*

References:

1. A. Szczes et al. *Advances in Colloid and Interface Science* **249** p. 321–330 (2017)
2. Y. Gou et al. *Nano TransMed* **3 p.** 100033 (2024)
3. H. Zhou et al. *Acta Biomaterialia* **127** p. 41–55 (2021)
4. V. Uskokovic et al. *Ceramics International* **46** p. 11443–11465 (2020)

POLYMERS AND COMPOSITES

P52 – P63

P52. Assessing the Performance of Small Concrete Beams Reinforced with Steel and Fiber Reinforced Polymer Bars

Abel Belay, Julita Krassowska, Marta Kosior-Kazberuk

Białystok University of Technology
Wiejska 45A 15-351, Białystok, Poland
abel.belay@sd.pb.edu.pl

This research investigates the performance of small concrete beams reinforced with glass fiber reinforced polymer (GFRP), basalt fiber reinforced polymer (BFRP), and traditional steel bars. It addresses limitations of steel reinforcement and explores alternative strategies for better infrastructure solutions. FRP materials offer benefits like lightweight properties, cost-effectiveness and corrosion resistance. The study analyzes strength, load-bearing capacity, failure modes, and deflection of concrete beams reinforced with these materials.

Concrete beams were prepared with CEM I 42.5R Portland cement, a water-cement ratio of 0.5, sand, aggregates, and super-plasticizer. Reinforcements included 6 mm diameter S-500 steel bars, 6 mm BFRPs, and 8 mm GFRPs, all 940 mm long. An experimental program assessed the ultimate load-bearing capacity, mid-span deflection, average deformation, and failure modes. Specimens' concrete were mixed, cured, and tested per Eurocode. Six beams (120 × 80 × 1100 mm) with steel, GFRP, and BFRP reinforcements were used.

GFRP-reinforced beams supported higher ultimate loads than BFRP and steel-reinforced beams. BFRP beams, despite early crack initiation, had higher ultimate load-bearing capacity than steel beams.

Steel reinforced concrete beams failed at 20 KN and 21.8 KN with mid-span deflections of 4.76 mm and 4.65 mm. GFRP reinforced concrete beams failed at 32 KN and 40 KN, with deflections of 14.01 mm and 14.61 mm. BFRP reinforced concrete beams failed at 26 KN and 30 KN, with deflections of 16.17 mm and 21.50 mm. GFRP reinforced concrete beams had significant deformations and larger crack widths. Failure modes differed: steel beams had flexural tension failure, GFRP beams had diagonal tension leading to shear tension failure, and BFRP beams had combined diagonal tension and flexural failure.

This research highlights a shift towards using GFRP and BFRP materials in concrete beams, comparing their mechanical characteristics and effectiveness against traditional steel reinforcement under concrete beams.

Keywords: *BFRP, GFRP, Steel bars and Concrete beams.*

P53. Exploring PV Module Structures Combining Conventional Building Elements and PV Module Materials

Algirdas Baležentis[1,2], Piotr Dubravskij[2], Eglė Fataraitė-Urbonienė[2,3], Juras Ulbikas[1,2], Jolanta Donėlienė[2], Matas Rudzikas[2]

[1]JSC Modern E-Technologies, Vismaliuku St. 34, LT-10243 Vilnius, Lithuania
[2]Applied Research Institute for Prospective Technologies, Vismaliuku St. 34, LT-10243 Vilnius, Lithuania
[3]Kaunas University of Technology, K. Donelaicio St. 73, LT-44249 Kaunas, Lithuania
Algirdas@met.lt

In the Building Integrated Photovoltaics (BIPV) sector, a common practice involves the use of standard glass/glass-based PV modules. While these technologies offer reliability, their installation typically demands additional fixings and specialized, costly installation expertise. Therefore, there's a need for a new generation of photovoltaic modules - ones that combine conventional construction materials with those used in photovoltaics to provide an aesthetic solution and reduce installation costs, as they would require the same fixings as conventional facade elements.

This study aims to identify the most effective combinations of construction elements and PV materials and maintain acceptable adhesion properties between the PV encapsulation material and facade material to ensure the durability and longevity of the technology. Various material combinations (refer to fig. 1) have been tested as part of the research process.

Most promising results were achieved using: 1) Glass front layer, Ethylene-vinyl acetate (EVA) encapsulant, steel roof coated with polyester as a back layer; 2) Glass front layer, Ethylene-vinyl acetate (EVA) encapsulant, steel roof coated with powder coating as a back layer; 3) copolymer of ethylene tetrafluoroethylene (ETFE) front layer, Ethylene-vinyl acetate (EVA) encapsulant, coated with polyvinylidene fluoride PVDF aluminium facade sheet as a back layer.

These samples were tested according to the IEC 61215 standard in order to determine their durability. All structures were placed in the climatic chamber and subjected to the "Damp Heat" test, which involved exposing them to a temperature of 85°C and a relative humidity of 85% for a duration of 500 hours. After the test, a visual inspection was performed, and no delamination was found. In addition, both PV structures were tested with adhesion tests, which showed a decrease in adhesion from 41.18% to 74.39%, depending on the number of layers of material used. It was found that some of the conventional facade materials can be laminated with standard PV module materials.

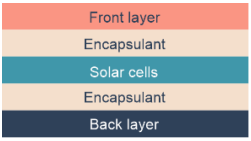

Fig. 1. Front layers – ETFE, glass; encapsulation materials – EVA and POE; back layers – steel roof coated with polyester, steel roof coated with polyester, powder coated steel roof, coated with PVDF aluminium facade sheet

Keywords: *Building Integrated Photovoltaics, back layer, front layer, encapsulant, new generation PV modules, adhesion, facade materials.*

P54. High Hydrostatic Pressure as a Prospective Approach for Processing and Sterilizing Drug-loaded Hydrogels

Anete Vircava[1,2], Agnese Brangule[1,2], Ingus Skadiņš [2,3]

[1]Department of Pharmaceutical Chemistry, Riga Stradinš University, LV-1007 Riga, Latvia
[2]Baltic Biomaterials Centre of Excellence, Headquarters at Riga Technical University, LV-1658 Riga, Latvia
[3]Department of Biology and Microbiology, Rīga Stradiņš University, Dzirciema St. 16, LV-1007 Riga, Latvia

Hydrogel-based biomaterials find widespread application in biomedicine, serving as scaffolds in tissue engineering, wound dressings, drug delivery systems, and contact lenses [1]. Despite their promising properties in biomedicine, it is crucial to address production and sterilization challenges for hydrogels, as their water content makes them sensitive to traditional sterilization methods [2]. High Hydrostatic Pressure (HHP) stands as a potent alternative to conventional sterilization methods, such as high-temperature thermal processing, steam-based methods, gamma irradiation, and chemical agents. Additionally, the HHP technique serves as a dual-purpose method, applicable during both the hydrogel preparation stage and sterilization process [3]. The HHP process involves various parameters and variables, which contribute to its complexity. Therefore, the study employs an innovative Artificial Intelligence/Machine Learning (AI/ML) algorithm for process optimization.

The aim of this project is to design drug-loaded hydrogel with enhanced pharmaceutical properties using the HHP processing method.

In the study, various HHP sterilization conditions, including time (5–15 min), pressure (100–300 MPa), and cycles (1–4), were tested for effectiveness against *E.coli* bacteria. Our experiment and ML approach showed that a pressure of 200 MPa, 2–4 cycles, and 10 minutes of pressure holding can effectively deactivate microbiological samples. This strategy has the potential to optimize multi-parameter processes and improve drug-loaded hydrogels, ultimately leading to better medical outcomes.

Acknowledgements: The project "RSU internal and RSU with LSPA external consolidation", No. 5.2.1.1.i.0/2/24/I/CFLA/005; Researcher Grant “High Hydrostatic Pressure: A Dual-Function Method for Processing and Sterilizing Drug-Loaded Hydrogels”, No. RSU-ZG-2024/1-0002.

Keywords*: high hydrostatic pressure, sterilization, hydrogel, bacteria, Machine Learning*.

References:

1. E. Calo et. al. *European Polymer Journal* ***65*** p. 252–267 (2015)
2. R. Galante et.al. *Journal of Biomedical Materials Research Part B: Applied Biomaterials* **106(6)** p. 2472–2492 (2018)
3. D. Larrea-Wachtendorff et. al. *Gels* **8(3)** 152 (2022)

P55. Evaluation of Polymer Gel Dosimeters Response to Electron and X-ray Irradiation: Dependence of Dose Rate and Energy

Aurimas Krauleidis[1,2], Diana Adlienė[1]

[1]Kaunas University of Technology, Department of Physics, Studentų St. 50, LT-51368 Kaunas, Lithuania
[2]Klaipėda University Hospital, Liepojos st. 41, LT-92288 Klaipėda, Lithuania
aurimas.krauleidis@ktu.edu

The photon and electron-induced radical-initiated polymerization in polymer gels can be used to construct high-resolution tissue equivalent dosimeters for radiation therapy quality control. The dose distribution in irradiated gel dosimeters reflects changes in molecular mobility caused by local polymerization initiated by radiation-generated radicals. It can be assessed by analyzing magnetic resonance or X-ray CT imaging parameters [1,2]. Physical factors, such as dose rate and energy are responsible for the dosimetric sensitivity of gel dosimeters [3].

Several types of gel dosimeters were prepared and analyzed: normoxic methacrylic acid gel (nMAG), normoxic polyacrylamide gel (nPAG), and N-isopropyl acrylamide gel (NIPAM).

Fabricated gel dosimeters were irradiated with 6 MeV and 15 MeV photon or electron beams applying different dose rates (100, 300, and 600 cGy/min). Dose-related MRI relaxation rate R2, and CT number changes of the irradiated gels were analyzed [4].

It is known [5], that the dosimetric sensitivity of the gel dosimeters to irradiation is defined by the slope of the calibration curve obtained for each evaluating modality separately. It was found that the dose-response of gels was similar for both irradiation beams (photons and electrons) in the lower dose range up to 5 Gy indicating high sensitivity to dose rate and beam energy changes. The dose sensitivity of the gels was highly dependent on the dose rate and beam energy used.

Performed investigation revealed that nMAg gel was more sensitive to dose rate and beam energy changes as compared with nPAG or NIPAM gels.

Keywords: *dose rate, dosimetry, energy, gels.*

References:

1. M. Khan et al*. Polymers* **11(10)** p. 1717 (2019)
2. H. Borujeini et al. *Appl. Magn. Reson*. **52** p. 1671–1687 (2021)
3. S. M. M. Abtahi et al. *Radiat. Phys. Chem*. **172** 108784 (2020)
4. V. Anaraki et al. *Radiat. Phys. Chem*. **153** p. 35–43 (2018)
5. M. Merkis et al. *Polymers* **13(22)** p. 3925 (2021)

P56. Physicochemical Properties of Choline Chloride-based Deep Eutectic Solvents

Paulina Nemaniutė, Asta Grigucevičienė, Dalia Bražinskienė

Center for Physical Sciences and Technology (FTMC), Saulėtekio Ave. 3, LT-10257 Vilnius, Lithuania
dalia.brazinskiene@ftmc.lt

Chemical stability and environmental friendliness are two of the most important features of deep eutectic solvents (DES). The materials that make up their structures are readily available, inexpensive, non-toxic, biodegradable and non-flammable [1]. Since the deep eutectic phenomenon was introduced in 2003 [1], choline (2-hydroxyethyl-trimethylammonium) chloride has been the subject of the most research. DES of choline chloride has been used both for the efficient recovery of raw materials from used Li-ion batteries [2,3], for their applications in food packaging [4], and for the recycling of non-degradable polyurethanes [5].

Although this is economically and environmentally advantageous, existing technologies still face practical problems. DES of choline-chloride are becoming increasingly important for industrial applications and new scientific developments in their physical and chemical properties are expected. As a result, it's critical to consider characteristics like stability, degradation, fluidity, and viscosity when designing the optimal system for a particular application because these attributes are heavily influenced by the molecular composition of each system's constituent parts and their interactions with one another.

DES formulations have been prepared from choline chloride and various H-bond donors, such as urea, diphenyl urea, LD-malic acid and xylitol. The aim of this study was to evaluate their stability and phase equilibrium not only at ambient temperatures but also at higher temperatures. The oxidation resistance was evaluated using a thin-film method as described previously [6]. By applying thin films of DES to the steel surface at 90°C and following the gravimetric changes, their volatility and degradation patterns were studied. The DES tested had low evaporation rates and relatively high viscosity.

Acknowledgments: *This study was carried out under project TERMINUS, funded by the European Union under Horizon 2020. Call: H2020-MBP-ST-IND-2018. Grant Agreement: 814400.*

Keywords: *choline chloride, DES, viscosity, oxidative degradation.*

References:

1. A. P. Abbott et al. Green Chem. **13** p. 471–481 (2011)
2. Mai K. Tran et al. *Nature Energy.* **4** p. 339–345 (2019)
3. M. Jafari et. al. *J. Env. Chem. Eng.* **10(6)** p. 109014 (2022)
4. A. C. Galvis-Sá nchez et al. *Food Hydro-colloids* **82** p. 478−489 (2018)
5. H. Zhang et al. *Polymer Degradation and stability* **181** p. 109342 (2020)
6. Liascukiene et al. *Fuel Processing Technology* **180** p. 87–95 (2018)

P57. Comparison of Surface Roughness Parameters of Abraded Polymer Materials of Different Softness

Yadukrishna Kandamkarikkal Murali[1], Joris Vėžys[1], Jolanta Donėlienė[2], Eglė Fataraitė Urbonienė[1,2]

[1]Kaunas University of Technology, K. Donelaičio St. 73, LT-44029 Kaunas, Lithuania
[2]The Applied Research Institute for Prospective Technologies, Vismaliukų St. 34, LT-10243 Vilnius, Lithuania
egle.fataraite@ktu.lt

The adhesive joining of materials of different natures allows using a wide variety of materials, not only offering great design flexibility, compared to traditional mechanical fastening methods but also resulting in more even stress distribution, reducing the risk of high-stress concentration zones, which can lead to material damage, enhance performance in extreme condition etc. Among many factors influencing adhesion, surface characteristics such as surface energy, surface cleanliness, surface roughness, and materials' chemical and mechanical properties are the most important.

The investigation aimed to evaluate the influence of polymer material softness and abrasion conditions on the surface roughness parameters.

Four types of soft polymer materials (E < 300 MPa) were selected for investigation: two types of monolithic vulcanized rubber, butadiene-styrene rubber, and microporous material – ethylene vinyl acetate (EVA) copolymer. The surface of the tested materials was roughened using two different abrasives grade numbers No 60 and No 100. Shore hardness A of materials was measured using a digital hardness meter and the profiles before and after surface abrasion were carried out using portable surface roughness tester Mitutoyo Surftest SJ-210, and the optical micrographs were obtained using Mitutoyo quick vision device QV-404.

It was determined that statistical surface roughness parameters are in high dependence not only on the abrasive paper grade number but also depends on the materials softness and porosity. For the nonporous polymer materials with Shore hardness A close to 90 a. u. very clear dependence of abrasive paper grade number was found. The surface roughness after abrasion was increased several times compared with a non-abraded surface, while for nonporous rubber with Shore hardness A equal to 60 a. u. and microporous EVA samples, this effect was not so evident. It was not found a significant influence of abrasive paper grade number on the surface roughness of the material. The difference between Ra values was not higher than 25% when the surface was roughened with abrasive paper No60 and No100.

Keywords: *surface roughness, rubber, abrasion.*

P58. BIO4EEB – BIO Insulation Materials for Enhancing the Energy Performance of Buildings

Vitas Mačiulis, Eglė Fataraitė-Urbonienė, Saulius Pakalka

The Applied Research Institute for Prospective Technologies, Vismaliukų St. 34, LT-10243 Vilnius, Lithuania
egle.fataraite@ktu.lt

Buildings are responsible for approximately 40% of energy consumption and 36% of CO_2 emissions in the EU. Deep renovation of existing old buildings has the potential to lead to significant energy savings and a tremendous carbon footprint shrinkage. The current EU climate targets open an ample opportunity for exponential growth in the building thermal insulation materials market owing to the increasing number of new residential buildings and current deep renovation needs.

The target of BIO4EEB project (https://www.bio4eeb.eu/), is to support residential building´s construction performance extraordinary at all three hierarchical levels of construction parts simultaneously (building, component, material) by creating an amplified environmental impact and reducing additionally VOC emissions. BIO4EEB applying non-hazardous bio-based material as e.g., Posidonia and various bio-based foams to develop and to proof the marketability of smart components for external and internal use as material application, pre-fab panels or windows. The efficiency and effectiveness is quite important to match with market demands and establish a unique selling proposition including a seven years return on investment.

BIO4EEB seeks to close the increasing gap of insulation material shortage caused by the regular growing demand and the mismatch caused by lacking production potential and the outcome of the current energy crisis by boosting the use of available bio-based qualified materials as alternative solutions. The objective is to substitute using fossil resources for components and replace them at a comparable price value positioning. New business models utilizing the complete economic value chain open the market for bio-based BIO4EEB solutions and products uplifting the generic bio-based material use and qualifying their application at a circular economy approach for creating a much greener EU building and construction industry real estate stock.

***Acknowledgments*:** This project received funding from the European Unions‘s Horizon Europe research and innovation program under grant agreement N°101091967.

Keywords: *materials engineering, bio-based materials, thermal insulation.*

P59. Product Authentication with Active Optical Elements and Special-Purpose Dyes

Indrė Danisevičienė, Erika Rajackaitė, Andrius Žutautas, Pranas Narmontas

Institute of Materials Science, Kaunas University of Technology,
K. Baršausko St. 59, LT-51423 Kaunas, Lithuania
indre.daniseviciene@ktu.lt

The essence of the research is to present a new multifunctional product labeling system to the market. Polygraphic technologies, physicochemical synthesis and analysis methods were used for its creation. This system allows to identify objects and determine their origin. The newly developed labeling system ensures the highest level of protection against counterfeiting, creates the possibility of automating trade and logistics systems, and also contributes to the implementation of the goals of the circular economy by integrating it into new deposit systems in order to increase the collection of recyclable waste, etc.

An optical diffraction marks of periodic structures of variable period, also called holographic meta-surfaces, characterized by dynamic changes in the shape, size, position and color of optical elements depending on the amplitude, phase, polarization, wavelength of light, spatial position of the light source relative to the mark and the observation point of the observer, were created. Dynamic motion security marks (active optical elements) and special-purpose dyes have been developed and integrated into the marking system, which guarantee a high level of protection against forgery.

Keywords: *active optical elements, special-purpose dyes, security, authentication.*

References:

1. J. Žiljak Gršić et al. *Information* **13(2)** p. 47 (2022)
2. J. Ž. Gršić et al. *Applied Sciences* **12(4)** p. 2152 (2022)
3. Jianhua Mei et al. *Critical Reviews in Food Science and Nutrition* **62(23)** p. 6374–6389 (2022)
4. Yunxiang Lei et al. *A Journal of the German Chemical Society* **59(37)** p. 16054–16060 (2020)

P60. Polymer Films with Green Silver Nanoparticles from Symphyti Radix as Antibiotic Oxidants

Khadija Ramzan, Jonas Viskelis

Institute of Horticulture, Lithuania Research Center for Agriculture and Forestery, Kauno St. 30, LT-54333 Kaunas, Lithuania
khadija.ramzan@lammc.lt

Antibiotic-resistant microorganisms are posing serious global health risks due to their growth and distribution. Organic substance has varied chemical composition and mode of actions due to which they have strong potential to fight against microbial disease. Among all of them silver nanoparticles (AgNPs) have shown exceptional antibacterial capabilities, which has led to their investigation in a range of industrial and biological uses. The aim of this study to use of aquatic plant root extracts for the biosynthesis of silver nanoparticles (AgNPs) as minimizing coatings and film formatting in antimicrobial natural polymer film. Transmission electron microscopy (TEM) and scanning electron microscopy–energy-dispersive spectroscopy (SEM–EDS) methods were used to validate the production of polymers. Using the Kirby-Bauer disk diffusion susceptibility test to investigate the growth of Gram-positive and Gram-negative bacterial cultures. The antioxidant activity and antibacterial activity of biofilm containing green AgNPs was also examined. From results we get that total phenolic content were slightly higher in aqueous extracts of Sym. Radix than in Sym. Radix/AgNPs. AgNPs were shown to include spherically shaped nano-objects with an average size of 27.45 nm in TEM images. Studies of the surface morphological indicated that the films' acquired surface was smooth and free of any holes or other imperfections in the relief. In the age of multi-drug resistance, these apparent biological functions of AgNPs and Symphyti radix polymer film may offer a platform for combating harmful microorganisms.

Keywords: *green synthesis, Symphyti radix, silver nanoparticles, phytochemical analysis, antibacterial activity, antioxidant activity.*

References:

1. N. Dey et al. *A review. Environ. Res.* **214** p. 113867 (2022)
2. Z. W. Taye et al. *Front. Public Health* **11** p. 1087407 (2023)
3. E. Efstratiou et al. *Complement. Ther. Clin. Pract.* **18** p. 173–176 (2012)
4. D. Ding et al. *Ecotoxicol Environ Saf.* **254** p. 114734 (2023)

P61. Application of Nanocomposites to Remove Micro and Nanoplastics

Mahrosh Javed, Galina Lujanienė, Sergej Šemčuk, Vidas Pakštas, Kęstutis Mažeika, Algirdas Selskis

SRI Center for Physical Sciences and Technology, Savanorių Ave. 231, Vilnius, Lithuania
mahrosh.javed@ftmc.lt

New data on the presence of micro- and nanoparticles in various Earth environments such as air, water, soil, and wildlife, including the tissues and gastrointestinal tracts of thousands of animal species, as well as in human tissues and fluids, are raising growing concerns about plastic pollution. New methods for analysing nano- and micro-plastics (MNPs) and reusing old technologies have been developed, making it possible to determine the extent and magnitude of plastic pollution down to the nanoscale (< 1 μm). However, there are only a limited number of studies on NMPs from real-life derived samples in the < 1 μm range. Most studies in this range have been conducted with polystyrene (PS) plastics, as micro-nanospheres made from other plastics are not commercially available. In addition, recent studies have shown that real-life plastic particles exhibit different behaviour than chemically pure plastics. Recently published new protocols to produce real NMP samples under laboratory conditions have made it possible to produce NMPs in the laboratory and use them for various experiments.

This study has aimed to prepare polyethylene terephthalate (PET) NMPs of < 1 μm from real-life plastics such as single-use water bottles and use them in adsorption experiments. NMPs were prepared using mechanical fragmentation, and milling (using ball mill Pulverisette 6 (FRITSCH, Germany). Characterization of obtained particles was performed using TEM, SEM, XRD, and FTIR.

Chitosan-graphene oxide (GO-CS) based nanocomposites were used as adsorbents for PET-NMPs and all changes resulting from the adsorption process were monitored by SEM, TEM, FTIR, XRD and Raman spectroscopy.

Keywords: *nano- and micro-plastics, chitosan-graphene oxide nanocomposites adsorption, fresh water.*

P62. Magnetic Biopolymers for Removal of Radionuclides and Emerging Contaminants in Aquatic Ecosystems

Sergej Šemčuk[1,2], Danguolė Montvydienė[1], Nijolė Kazlauskienė[1], Vidas Pakštas[2], Kęstutis Mažeika[2], Mahrosh Javed[2], Galina Lujanienė[2], Kęstutis Jokšas[1], Živilė Jurgelėnė[1]

[1]Laboratory of Ecotoxicology, Nature Research Centre, Akademijos St. 2, Vilnius, Lithuania
[2]SRI Center for Physical Sciences and Technology, Savanorių Ave. 231, Vilnius, Lithuania
sergej.semcuk@gmail.com

Natural resources such as water are constantly exposed to anthropogenic pollution. Various pollutants such as heavy metals (Zn, Ni, Cr, Hg, Cd, Cu, etc.), organic compounds (fertilizers, pesticides, phenols, organic dyes, pharmaceuticals, surfactants, etc.), and, above all, radionuclides (Eu, Co, Cs, etc.) can enter drinking water through the discharge of industrial wastewater. They are all highly toxic, non-biodegradable, have a higher solubility and mobility in water systems, and ultimately pose a threat to animal health and consequently to human health [1]. Among all technologies (such as sedimentation, flocculation, evaporation, membrane technology, etc.) used to purify contaminated water, the adsorption technique on suitable nanoporous or micro-/nanoscale materials such as activated carbon, zeolites, sol-gel routes, polymers, microemulsions, functionalized silica and clay, etc. is still considered one of the most effective and simplest. Recently, biopolymers such as chitosan are considered as important candidates for water treatment due to their non-toxicity, biodegradability, natural occurrence, considerable recovery rates, regenerative ability, and biocompatibility. Moreover, chitosan is a unique and modifiable material that can be used as a sorbent that has been modified with nanocomposites to give it additional capabilities such as magnetism (using Fe_2O_3) for rapid separation from water for recovery [2]. The potential of magnetic biopolymers for the removal of radionuclides and other emerging contaminants was investigated in this study. The SEM, TEM, FTIR, AFM, XRD, Raman, and Mössbauer methods were used for the characterization of the synthesized magnetic biopolymers and their changes during sorption. Furthermore, this research aims to perform a comprehensive evaluation of the direct effects of these nano-adsorbents on aquatic organisms to assess their ecological safety. The experiments confirmed the hypothesis that magnetic biopolymers used as sorbents attenuate the toxic effects (mortality, morphophysiological changes) of emerging pollutants on aquatic organisms (crustaceans and fish). The study combined adsorption efficiency with ecotoxicity assessment to gain valuable insights into the sustainable use of nano-adsorbents for water remediation. The obtained results will be useful for the effective removal of radionuclides and other emerging pollutants while protecting the environment and human health.

Acknowledgements: This work was funded by the Research Council of Lithuania, Project No. P-PD-23-187 “Fish as trophic ontogenesis model for studying the impact mechanisms of ecofriendly sorbents modified with nanocomposites”.

Keywords: *magnetic biopolymers, radionuclide sorption, nanocomposites, fish, crustaceans, biological parameters.*

References:

1. M. A. Ahmed et al. *Int. J. of Biological Macromolecules* **242(2)** p. 124787 (2023)
2. M. Shahadat et al. *Polymer* **254** p. 124975 (2022)

P63. Development of an Electrochemical Sensor Utilising Molecularly Imprinted Polypyrrole for the Rapid Detection of *Listeria monocytogenes* Bacteria

Viktorija Liustrovaite[1], Maksym Pogorielov[2, 3], Raimonda Boguzaite[1,4], Vilma Ratautaite[1,4], Almira Ramanaviciene[1], Greta Pilvenyte[4], Viktoriia Holubnycha[2], Viktoriia Korniienko[2,3], Kateryna Diedkova[2,3], Roman Viter[3], Arunas Ramanavicius[1,4]

[1]NanoTechnas–Center of Nanotechnology and Materials Science, Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Naugarduko St. 24, LT-03225 Vilnius, Lithuania
[2]Biomedical Research Centre, Sumy State University, R-Korsakova Street, 40007 Sumy, Ukraine
[3]Institute of Atomic Physics and Spectroscopy, University of Latvia, Jelgavas Iela 3, LV-1004 Riga, Latvia
[4]Department of Nanotechnology, State Research Institute Center for Physical Sciences and Technology, Saulėtekio Ave. 3, LT-10257 Vilnius, Lithuania
viktorija.liustrovaite@chgf.vu.lt

Listeria monocytogenes bacteria poses a significant threat to food safety, leading to severe infections and high mortality rates. In response to this challenge, molecularly imprinted polymers (MIPs) have emerged as promising candidates for the recognition of specific analytes due to their exceptional selectivity. The molecular imprinting approach involves creating binding sites uniquely suited to a specific molecule, leveraging the concept of complementarity between imprinted sites and the analyte [2].

In this study, we present a novel approach to developing a molecularly imprinted polypyrrole sensor (MIP-Ppy) for the rapid and selective detection of *Listeria monocytogenes* [3]. A distinctive aspect of this research involves evaluating efficient extraction methods for *Listeria monocytogenes* from imprinted cavities. The analytical performance of electrodes modified with a non-imprinted polypyrrole (NIP-Ppy) layer was compared with those modified by the MIP-Ppy layer.

The results demonstrate the selectivity of the MIP-Ppy sensor, offering a promising solution for the rapid and precise detection of *Listeria monocytogenes* in food samples. Sensitivity criteria, including the limit of detection (LOD) and limit of quantification (LOQ), were used to assess the performance, along with repeatability measurements. This electrochemical approach has great potential to advance *Listeria monocytogenes* detection in both healthcare and the food industry, providing a reliable and efficient solution to address this public health concern.

Keywords: *molecularly imprinted polymers, Listeria monocytogenes, bacteria.*
References:
1. V. Ratautaite et al. *Electrochimica acta* **403** p. 139581 (2022)
2. V. Liustrovaitė et al. *Polymers* **15(7)** p. 1597 (2023)

ADVANCED ENGINEERING MATERIALS

P64 – P70

P64. Revolutionizing Infrastructure Monitoring: Smart Cement and Sensor Integration

Addisu Solomon, Maria Ratajczak

Faculty of Civil Engineering and transport Poznań University of Technology, plac Marii Skłodowskiej-Curie 5, 60-965 Poznań, Poland
addisu.solomon@student.put.poznan.pl

The integration of smart cement and sensor technologies offers a unique opportunity to unify the approach to the remote monitoring and maintenance of infrastructure. Smart cement, which is enhanced with embedded sensors, represents a significant advancement in civil engineering materials, enabling real-time monitoring of critical structural parameters.

The integration of sensors within the cement matrix allows for continuous monitoring of factors such as strain, temperature, humidity, and corrosion levels. This real-time data collection provides engineers with valuable insights into the structural health and performance of infrastructure assets, facilitating early detection of defects and proactive maintenance interventions.

Furthermore, wireless communication technologies enable remote access to sensor data, empowering engineers to monitor infrastructure conditions from anywhere in the world. This connectivity facilitates timely decision-making, optimized maintenance schedules, and improved resource allocation, ultimately leading to enhanced infrastructure resilience and longevity.

In addition to real-time monitoring capabilities, the integration of smart cement and sensors opens avenues for advanced data analytics techniques. Machine learning algorithms can analyse large datasets collected from sensors to predict structural behaviour, identify patterns, and optimize maintenance strategies, thereby maximizing infrastructure performance and minimizing downtime.

Keywords: *smart cement, sensor integration, real-time monitoring, infrastructure resilience.*

P65. Green Synthesis of Silver Nanoparticles: A Promising Approach for Medical Applications

Akvilė Andziukevičiūtė-Jankūnienė[1], Erika Adomavičiūtė[1], Aistė Balčiūnaitienė[2], Virginija Jankauskaitė[1]

[1]Mechanical Engineering and Design Faculty, Kaunas University of Technology, Studentu St. 56, LT-51423 Kaunas, Lithuania
[2]Lithuanian Research Centre for Agriculture and Forestry, Institute of Horticulture, 54333 Babtai, Lithuania
akvile.andziukeviciute-jankuniene@ktu.lt

Silver nanoparticles (AgNPs) are of significant interest for their unique properties and medical potential. Conventional synthesis methods are energy-intensive and hazardous, while plant-based alternatives, leveraging phytochemical-rich extracts, offer safer, sustainable routes. However, biosynthesis methods often entail complexities in control, as they rely heavily on the biochemistry of the selected plant species. This study aims to develop a green AgNPs synthesis using *Chamomilla matricaria* (*ChM*) extract. Aqueous extract of *ChM* was prepared using a precursor $AgNO_3$ solution of different concentrations (c = 2–10 mM). The colour change of solution from yellowish to reddish brown visually evidences the formation of *ChM*-AgNPs (fig. 1a). It was confirmed by UV-Vis analysis (fig. 1b) – LSPR peak at 438 nm appear the bioreduction of Ag^+ ions to Ag^0 by phytochemicals. However, higher $AgNO_3$ concentrations exceeded optimal nucleation conditions, leading to Ag^+ ions aggregation rather than nanoparticles formation due to elevated ionic strength and excess silver ions [1]. TEM imaging (fig. 1c) showed spherical AgNPs with diameters 10–85 nm (average size of 32 nm), possibly due to variations in nucleation, growth kinetics, and inherent aggregation tendencies during synthesis.

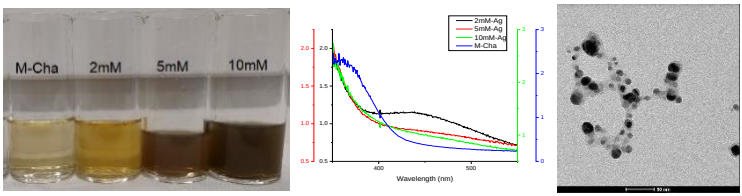

Fig. 1. Biosynthesized AgNPs investigation: a – *ChM* extract colour change after 1 h, b – UV-Vis absorption spectra, c –TEM image of AgNPs

Spherical AgNPs were successfully obtained using *Chamomilla matricaria* aqueous extract. Nevertheless, optimizing the herbal extract and $AgNO_3$ concentrations is crucial to ensure AgNPs stability, size uniformity, and preventing aggregation.

Keywords: *silver nanoparticles, green synthesis, Chamomilla matricaria.*

References:

1. T. Yin et al. *Journal of Membrane Science* **449** p. 9–14 (2014)

P66. Peculiarities in Growing Thin Film Multilayer Nanostructures for Applications in Giant Magnetoresistance – Based Sensors

Dariuš Antonovič, Vilius Vertelis, Andrius Maneikis, Nerija Žurauskienė

Center for Physical Sciences and Technology, Saulėtekio Ave. 3, LT–10257 Vilnius, Lithuania
darius.antonovic@ftmc.lt

Giant magnetoresistance (GMR) effect can be described as the change in the electric conductivity of a multilayer structure, usually consisting of two ferromagnetic layers separated by a non – magnetic conductive layer, when an external magnetic field changes the magnetization directions of the ferromagnetic layers relative to each other. A parallel alignment usually has a lower resistance than an antiparallel alignment [1]. High sensitivity to small changes in magnetic field strength makes GMR structures very attractive for sensor applications in medicine and informational technologies.

However, the ferromagnetic layers can also be separated by a thin insulating layer, which leads to the creation of a magnetic tunnel junction (MTJ). These structures exhibit an effect that is an extension of the GMR effect – tunnel magnetoresistance (TMR). Electrons can cross the insulating layer via quantum tunnelling. The probability of tunnelling is higher when the magnetization of the ferromagnetic layers is aligned in parallel and the lowest at an antiparallel alignment [2].

Various thin film technologies can be used to grow multilayer structures. In our research the main focus was on the magnetron sputtering (MS) technique and pulsed laser deposition (PLD) systems. Structure characterization was achieved by placing samples in a uniform magnetic field generated by an electromagnet and measuring changes in resistance induced by changes in magnetic flux density.

The goal of our research was to produce the GMR structures with engineered magnetoresistive properties. For this reason, we optimized the manufacturing process for efficient GMR structure production and investigated the magnetoresistive properties of the prepared devices.

Keywords: *thin films, giant magnetoresistance, tunnel magnetoresistance, magnetron sputtering, pulsed laser deposition, magnetoresistive sensors.*

References:

1. I. Ennen et al. *Sensors* ***16(6)*** p. 904 (2016)
2. C. Reig et al*. Magnetic Sensors and Devices* p. 35–64 (2017)

P67. Nitrocellulose Membrane Modified with Flow-Delay Laser μ-Machined as a Sensitivity and Signal Enhancement Strategy

Gazy Khatmi[1], Tomas Klinavičius[2], Martynas Simanavičius[4], Laimis Silimavičius [3,4], Asta Tamulevičienė[1,2], Agnė Rimkutė[4], Indrė Kučinskaitė-Kodzė[4], Gintautas Gylys[3], Tomas Tamulevičius[1,2]

[1]Department of Physics, Kaunas University of Technology, Lithuania
[2]Institute of Materials Science, Kaunas University of Technology, Lithuania
[3]UAB Sanpharm, Lithuania
[4]Institute of Biotechnology, Life Sciences Center, Vilnius University, Lithuania
gazy.khatmi@ktu.edu, tomas.tamulevicius@ktu.lt

Nitrocellulose membranes are widely used in lateral-flow immunoassays (LFA) for different purposes diagnostic tests. The analyte fluid sample added to the membrane flows through the LFA by capillary forces, interacting with the detection of antibody-labeled gold nanoparticles [1–4].

Although its simplicity and practicality make it an appealing solution, it remains a grand challenge to substantially enhance the colorimetric LFA sensitivity. The local flow rate constraints imposed in nitrocellulose (NC) membranes via a number of vertical femtosecond laser micromachined microchannels are important for prolonged specific binding interactions. Porous NC membrane surfaces were structured with different widths and densities μ-channels employing a second harmonic of the Yb:KGW femtosecond laser and sample XYZ translation over a microscope objective-focused laser beam. The influence of the microchannel parameters on the vertical wicking speed was evaluated from the video recordings. The obtained results indicated that μ-channel length, width, and density in NC membranes controllably increased the immunological reaction time between the analyte and the labeled antibody by 950%. Image analysis of the colorimetric indicators confirmed that the flow rate delaying strategy enhanced the signal sensitives by 40% compared with pristine NC LFA.

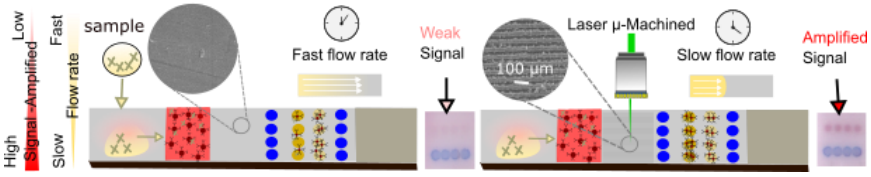

Fig. 1. Graphical abstract

Keywords: *nitrocellulose, μ-channels, laser μ-machining, reaction time, calorimetric sensing, signal enhancement.*

References:

1. N. G. Bastús et al. *Langmuir* **27** p. 11098–11105 (2011)
2. C. D. Skordoulis *Opt. Laser Technol.* p. 185–189 (1995)
3. I. Antanavičiūtė et al. *J. Tissue Eng. Regen. Med.* **12** p. e760–e773 (2018)
4. I. N. Katis et al. *Biosens Bioelectron* **113** p. 95–100 (2018)

P68. Enhancing Acoustic Properties of Wallboards Using Lignocellulosic Materials: Hemp Shives and Wood Chips

Ilze Gūtmane, Inga Zotova, Edgars Kirilovs

Institute of Arhitecture and Design, Riga Technical university,
6A Kipsalas Street, LV-1048 Riga, Latvia
inga.zotova@rtu.lv

Noise pollution is considered a stress factor that can adversely affect human health for a long time. Porous absorbing materials are used for passive control of various sounds and noises. Knowing the high porosity of technical hemp shives, it is essential to determine the acoustic properties of the manufactured board. The acoustic properties of the samples were described by determining whether the material is sound absorbent, by calculating the sound absorption and NRC coefficients, and by determining the absorption class.

Research is focused on establishing the optimal structure of wall panels to obtain a wall panel with high level of noise absorption. In the study, boards were made from hemp chips, wood chips and by mixing raw materials in a ratio of 50/50% to obtain a single-layer wall board with a thickness of 25±1 mm and a density of 225–20 kg/m^3. An impedance tube was used to measure the acoustic properties of the samples. Measurements were performed on 3 sample categories; a total of 18 samples were prepared and tested (see fig. 1).

All sample groups are sound absorbers with the highest absorption efficiency in the frequency band from 1000–2000 Hz and 4000–6300 Hz. Good sound absorption properties at frequencies 500–6300 Hz have the best absorption coefficient W 0.69 the porous structure of the board is able to improve the acoustic properties. Boards most effectively absorb sound in the frequency bands of 1000–2000 Hz and 4000–6300 Hz; corresponds to sound absorption class B and C (1000–4000 Hz). The NRC coefficient is determined at frequencies 250–2000 Hz. For the HW material group the coefficient is 0.47, for the H group it is 0.44, for the W group it is 0.49.

Fig. 1. Sound absorption samples (from left: HW; W; H)

Keywords: *hemp shive, wood chips, acoustic properties, optimal wallboard structure.*

P69. Geometric Distortion Analysis of Elements of QR Code Embedded in Textiles

Inga Breitmozerė[1], Jovita Dargienė[2], Jurgita Domskienė[1]

[1]Kaunas University of Technology, Faculty of Mechanical Engineering and Design, Studentų St. 56, LT-51424 Kaunas, Lithuania
[2]Kaunas College, Faculty of Arts and Education, Pramonės Pr. 20, LT-50468 Kaunas, Lithuania
inga.breitmozere@ktu.edu

QR codes are widely available, so they have become more popular in various industries, including textiles. Although there are significant challenges in integrating them into garments due to the features of textiles and QR codes.

Textiles are flexible and do not have a smooth surface owing to their structure, which is typically composed of woven or knitted threads. A wide variety of raw materials, from natural to man-made fibres, are used to make yarns. These characteristics strongly influence technologies that can be used to embed QR codes in textiles. On the other hand, for fluent QR code reading, it is essential that the image module configuration, positioning, and alignment markers [1,2] are not distorted because they are made of small elements (dots, squares) arranged in a grid. Therefore, the technologies chosen to realize QR on textiles must also be suitable to keep QR readability requirements. Furthermore, the applied QR codes could be breached during the garment lifecycle. Therefore, these aspects must be considered and tested.

The aim of the research is to assess the quality of embedded QR codes based on image analysis.

Investigations have been conducted on knitted polyester fabric using technologies such as heat transfer printing, sublimation, and embroidery to embed the QR code. An image analysis methodology was created to assess the quality and evaluate the readability of QR codes. The parameters of image similarity were chosen to compare the geometry of the QR code elements and to evaluate the image distortion. The results of QR image deformation in relation to the technologies used to embed QR codes on textile surfaces and the simulation of garment wearing conditions through abrasion and washing were obtained and described.

Keywords: *QR code, similarity, image analysis, geometric distortion.*

References:

1. J. Huang et al. *IET Image Processing* **14(13)** p. 3154–3160 (2020)
2. M. K. Teoh et al. *Computation* **10(9)** p. 147 (2022)

P70. Synthesis of Antiviral Silver Nanoparticle Polymer Nanocomposite Coatings with 3D Printing Integration for Long-lasting Antimicrobial Protection

Mindaugas Ilickas[1], Asta Guobienė[1], Brigita Abakevičienė[1,2]

[1]Institute of Materials Science, Kaunas University of Technology, K. Baršausko St. 59, 51423 Kaunas, Lithuania
[2]Department of Physics, Kaunas University of Technology, Studentų St. 50, 51368 Kaunas, Lithuania
mindaugas.ilickas@ktu.edu

Developing surfaces to combat viral diseases requires extensive research, money, and time due to the constant emergence of new pathogens. The recent threat of SARS-CoV-2 underscores the importance of new antimicrobial materials. A unique method involving UV-mediated photochemical synthesis has been introduced to produce silver-polymer (AgNP-PVB) nanocomposite coatings. These coatings are specifically designed to reduce the spread of diseases on frequently touched surfaces such as door handles, keypads, and elevator buttons.

Moreover, the size and concentration of AgNPs significantly affect the antiviral properties of these coatings. Comprehensive studies utilising techniques such as Raman spectroscopy, X-ray diffraction, atomic force microscopy (AFM), ultraviolet visible near-infrared spectroscopy, and contact angle (CA) measurements were carried out to analyse the characteristics of AgNP-PVB coatings. The effectiveness against viruses was assessed by testing SARS-CoV-2 RNA using a one-step qRT-PCR method.

The findings confirmed the presence of AgNPs within the PVB matrix with AFM analysis that revealed a decrease in the AgNP size as the irradiation duration increased. The results of the CA measurements showed a link between surface free energy (SFE) and antiviral effectiveness, indicating that higher levels of SFE were related to antiviral activity. Coatings containing 150, 200, 500 and 1000 ppm AgNP demonstrated reductions in the activity of SARS-CoV-2, hinting at their promise as preventive measures against viral infections.

A method has been developed that combines algorithms and 3D printing techniques to apply these coatings in the production of a door handle cover. This approach resulted in the successful development of a long-term, durable antiviral AgNP-PVB nanocomposite coating with varying AgNP sizes (ranging from 15 to 118 nm) and concentrations.

Keywords: *photochemical synthesis, silver nanoparticles, AgNP-PVB nanocomposite, antiviral activity, 3D printing.*

MATERIALS FOR ENERGY

P71 – P84

P71. Preparation of Platinum-Iron Nanoparticles Supported on Reduced Graphene Oxide by Using a Green-chemistry Method

Adriana Marinoiu

Institute for Cryogenics and Isotopic Technologies – ICSI, Uzinei St. 4, Ramnicu Valcea, Romania
adriana.marinoiu@icsi.ro

Platinum-iron nanoparticles supported on graphene oxide was synthesized by using a single-step synthesis microwave method in the presence of sodium borohydride, by employing a fast and eco-friendly microwave-assisted polyol process, which facilitated the simultaneous reduction of graphene oxide and formation of Pt nanocrystals.

The resultant doped-graphene oxide was demonstrated to act as an improved catalyst, as an electrode with a much better electrocatalytic activity, long-term operation stability, and tolerance to crossover effect than platinum for oxygen reduction *via* a four-electron pathway in fuel cells.

Among the fuels used, proton exchange fuel cells (PEMFCs) have been attracted considerable attention due to unique physical and chemical properties such as sustainable, ease of transportation and identified as the applicable fuel.

The structure and composition of the synthesized catalysts were examined by Fourier infrared spectroscopy, X-ray spectroscopy measurements XPS, specific surface area. The electrocatalytic activity of the synthesized catalysts toward the ORR was investigated by specific techniques, such as cyclic voltammetry, electrochemical impedance spectroscopy and I-V polarization curves.

The half-cell experiments revealed a higher ORR electrocatalytic activity. Electrochemical evaluation of platinum-iron doped-graphene oxide leads to significant improving of its functional characteristic in particular electrocatalytic activity in oxygen reduction reaction: well-defined cathode peaks for different scan rate and long term stability.

The important role of prepared catalyst for ORR can be applied to various carbon materials for the development of other metal efficient ORR catalysts for fuel cell applications, even new catalytic materials for applications beyond fuel cells.

Acknowledgements: This work was supported by Ministry of Research, Innovation, Digitization from Romania by the National Plan of R & D, Project No. PN 23 15 01 03, and by UEFISCDI, Contract No. 695PED/2022 (Project PN-III-P2-2.1-PED-2021-0840).

Keywords: *platinum-iron nanoparticles, graphene oxide, microwave.*

P72. Monolayers with Carbazole Moiety and Different Functional Groups for Perovskite Solar Cells

Aida Drevilkauskaite, Artiom Magomedov, Vytautas Getautis

Department of Organic Chemistry, Kaunas University of Technology, Radvilenų St. 19, LT-50254 Kaunas, Lithuania
aida.drevilkauskaite@ktu.lt

Inverted perovskite solar cells (iPSCs) are increasingly using self-assembled monolayers (SAMs) as hole-transporting materials due to their ease of formation and cost-effectiveness. A well-known example of SAMs is phosphonic acid with a carbazole moiety and various functional groups [1]. Despite promising results, the relationship between the molecular structure of SAMs and the electrical properties of iPSCs remains unclear. While it is well established in the literature that certain anchoring groups, like phosphonic acid, have the capability to form a monolayer with strong bonds on the surface of oxides, there is limited knowledge regarding how the position of functional groups in the chromophore impacts the properties of the monolayers (including wetting angle, surface passivation, work function fine-tuning) [2]. This study aims to understand how changes in the structure of SAM molecules relate to their electrical properties in photovoltaic devices. We synthesized and tested a series of molecules with phenyl functional groups as hole-transporting materials in iPSC devices. The results showed a significant impact of the phenyl substituent's position on the device efficiency. Specifically, phenyl substituents at the 3 and 6 positions of the carbazole moiety had efficiency similar to that of the well-known SAMs molecule, while substituents at the 4 positions resulted in lower efficiency. These findings underscore the importance of careful design and optimization in creating efficient hole-transporting materials for photovoltaic devices. Further research is underway to synthesize molecules with different functional groups and analyze their abilities to better understand how the position of functional groups on the carbazole moiety relates to photovoltaic device performance.

Keywords: *hole transporting material, self-assembled monolayer, perovskite solar cells.*

References:
1. A. Al-Ashouri et al. *Science* **370** p. 1300–1309 (2020)
2. S. A. Paniagua et al. *Chemical Reviews* **116** p. 7117–7158 (2016)

P73. Investigation of the Influence of Heavy Mg^{2+}-codoping on Emission Properties of $(Lu,Gd)_3(Ga,Al)_5O_{12}$:Ce Scintillators

Arnoldas Solovjovas[1], Saulius Nargelas[1], Yauheni Talochka[1], Žydrūnas Podlipskas[1], Miroslav Kucera[2], Zuzana Lucenicova[2], Gintautas Tamulaitis[1]

[1]Institute of Photonics and Nanotechnology, Vilnius University, Saulėtekio Ave. 3, LT-10257 Vilnius, Lithuania
[2]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, 12116 Prague, Czech Republic
arnoldas.solovjovas@ff.vu.lt

Fast timing characteristics of scintillators is essential in high energy physics and medical imaging fields. Cerium-activated garnet scintillators are currently among the most promising fast scintillators. The successful growth of Ce-doped gadolinium aluminium gallium garnet (GAGG) single crystals that are prospective for the detection of ionizing radiation encouraged a further development of mixed garnet-type scintillators for fast scintillating detectors. Recent studies show that the scintillation response time of Ce doped garnets might be improved by codoping with small amounts of divalent alkali-earth ions, usually Mg^{+2} or Ca^{+2}.

We present a study aimed at revealing the characteristics of recombination centers in heavily aliovalently codoped Ce-activated garnet-type scintillators. The investigation was conducted on a set of $Lu_{0.8}Gd_{2.2}Ga_{2.5}Al_{2.5}O_{12}$:Ce,Mg single crystalline epitaxial layers grown by isothermal dipping liquid phase epitaxy (LPE) on (100)-oriented Czochralski-grown $Gd_3Ga_{2.7}Al_{2.3}O_{12}$ substrates using BaO-B_2O_3-BaF_2 flux. LPE method allowed for a high concentration of codopant ions without substantial deterioration of the crystalline lattice. The content of aliovalent codopant Mg^{2+} in the investigated LuGAGG layers varied from 0 to 2200 ppm.

The influence of Mg^{2+} ions on the excitation relaxation and emission properties of Ce^{3+} activator ions in the set of LuGGAG:Ce layers was investigated using linear and transient absorption techniques, steady-state and time-resolved photoluminescence spectroscopy in the temperature range from 80 to 600 K.

The observed acceleration of Ce emission with increasing content of aliovalent codopant Mg^{2+} was interpreted by the coexistence of two types of emission centers: regular Ce^{3+} ions and Ce^{3+}+Mg^{2+} centers consisting of Ce ions located close to Mg ions. We found that magnesium has no effect on the energy position of the emitting $5d_1$ level of Ce^{3+}, however, Ce^{3+}-Mg^{2+} centers have a smaller energy barrier for thermal quenching and introduce a barrier-free channel of nonradiative recombination. Introduction of more magnesium results in a faster emission decay due to an increasing share of the Ce ions in the centers Ce^{3+}+Mg^{2+}.

Keywords: *scintillators, codoping, garnets.*

P74. Biofuel Cells Based on Metal Hexacyanoferrate Modified – Yeast Cells

Gabija Adomaitė, Aušra Valiūnienė

Institute of Chemistry, Vilnius University, Naugarduko St. 24, LT-03225 Vilnius, Lithuania
gabija.kavaliauskaite@chgf.stud.vu.lt

Yeast cells (*Saccharomyces cerevisiae*) are one of the most investigated cells [1]. Moreover, yeast cells are cost-friendly and easily available. For these reasons, many research works were introduced on yeast cell application in biofuel cells formations over the time [2–4].

In this research work, the yeast cell modification with metal hexacyanoferrates technique, which improves the yeast cells charge transfer parameters, is proposed. The modification impact on viability and electrochemical abilities of unmodified yeast cells and metal hexacyanoferrates – modified yeast cells are investigated. Furthermore, the metal hexacyanoferrate – modified yeast cell application in formation of biofuel cell is demonstrated and the principals of biofuel cells are introduced.

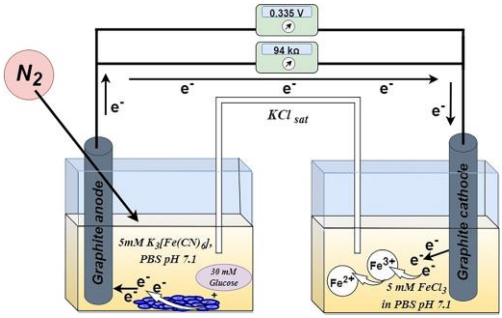

Fig. 1. Schematic representation of the biofuel cell based on PB-modified yeast [5]

Keywords: *yeast cells, biofuel cell, metal hexacyanoferrates.*

References:

1. G. Reed et al. *Yeast Technology*, The Avi Publishing Company, Westport, USA (1973)
2. A. Ramanavicius et al. *Fuel Cells* **9** p. 25–36 (2009)
3. Y. V. Hubenova et al. *Ind. Eng. Chem. Res.* **50** p. 557–564 (2011)
4. A. Halme et al. *IFAC Proc.* **28** p. 165–170 (1995)
5. G. Kavaliauskaitė et al. **928** p. 117079 (2023)

P75. Hydrogen Generation from an Alkaline $NaBH_4$ Solution Using Different Nickel Catalysts

Gitana Valeckytė, Zita Sukackienė, Virginija Kepenienė, Irena Stalnionienė, Vitalija Jasulaitienė, Jūratė Vaičiūnienė, Loreta Tamašauskaitė-Tamašiūnaitė, Giedrius Stalnionis, Eugenijus Norkus

Department of Catalysis, Center for Physical Sciences and Technology (FTMC), Saulėtekio Ave. 3, LT-10257 Vilnius, Lithuania
gitana.valeckyte@ftmc.lt

During this work, Ni/Cu, NiCo/Cu, NiMn/Cu, NiMo/Cu, NiCoMn/Cu, NiCoMo/Cu and NiCoMoMn/Cu catalysts were formed using the chemical method of metal deposition. The surface morphology, internal structure and chemical composition of the obtained catalysts were analysed using field emission scanning electron microscopy, X-ray photoelectron spectroscopy and induced plasma optical emission spectroscopy. It was determined that the prepared coating particles consist of oval-shaped agglomerates with a size of 40 nm to 1.6 μm. The studies of the composition of the catalysts showed that the Ni loading ranges from 32.515 to 475.15 μg/cm², Co – 346.65 to 614 μg/cm², Mn – 0.05 to 0.745 μg/cm² and Mo – 29.99 to 71.3 μg/cm². The catalytic properties of the formed catalysts for sodium borohydride hydrolysis reaction were investigated. The four-component NiCoMoMn coating was characterized by the highest catalytic activity. It was determined of this catalyst an activation energy of 45.3 kJ/mol and an H_2 evolution rate of 3.08 ml/min at 30°C and 23.57 ml/min at 70°C.

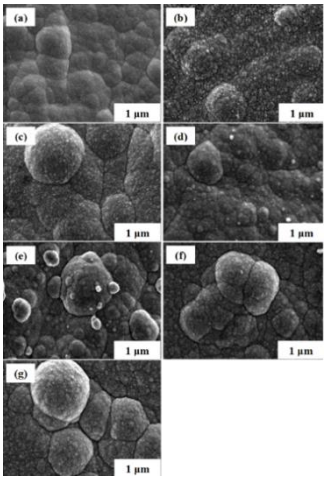

Fig. 1. FESEM images of prepared Ni/Cu (a), NiMn/Cu (b), NiMo/Cu /Cu (c), NiCo/Cu (d), NiCoMn/Cu (e) and NiCoMo/Cu (f), NiCoMoMn/Cu (g) catalysts

Keywords: *hydrogen, generation, nickel, cobalt, catalysts, borohydride.*

P76. Study of Fe_2O_3 and TiO_2 Molar Ratio Impact on Lithium-ion Battery Anode Performance

Kaspars Kaprans, Gunars Bajars, Gints Kucinskis

Institute of Solid-State Physics, University of Latvia, Riga, Latvia
kasparsk@cfi.lu.lv

Rapid development of portable electronic devices and electric vehicles demands for batteries with higher energy density, greater safety and longer cycle life. Transition metal oxide such as Fe_2O_3 has become a promising anode material for Li-ion batteries due to its high theoretical capacity and low cost [1]. However, the poor conductivity and violent volume expansion of Fe_2O_3 during the discharge/charge process results in its poor rate capability and cycling performance. The addition of TiO_2 prevents these problems because TiO_2 has good cycling stability and a low volume expansion ratio [2]. Therefore, a ternary Fe_2O_3/TiO_2/rGO anode material showed better electrochemical performance compared to the binary Fe_2O_3/rGO and TiO_2/rGO electrodes [3]. In this work, we study the Fe_2O_3 and TiO_2 molar ratio impact on lithium-ion battery anode performance.

The electrode materials of iron oxide, titanium dioxide and reduced graphene oxide (rGO) for lithium-ion batteries were prepared by electrophoretic deposition and their applicability was evaluated. A composition, structure and morphology of the electrode materials were investigated by scanning electron microscopy, atomic force microscopy, X-ray diffraction analysis, Raman spectroscopy, microspectral X-ray analysis and X-ray photoelectron spectroscopy.

In this study obtained gravimetric capacities of the ternary Fe_2O_3/TiO_2/rGO composite anode material at the discharge current 0.5 mA are 571, 683, 729 mAh/g for the nanocomposite electrode materials Fe_2O_3/TiO_2 in molar ratios of 1:1 (FT11), 2:1 (FT21) and 3:1 (FT31), respectively. After 400 charge-discharge cycles at the current value 1 mA, the nanocomposites retain 58%, 81% and 17% of its initial gravimetric capacity for FT11, FT21 and FT31, respectively. Based on the results of rate capability, cyclability and gravimetric capacity measurements, we conclude that the nanocomposite with a molar ratio of Fe_2O_3 to TiO_2 (2:1) has a potential as high-performance electrode material for lithium-ion batteries.

The results obtained in this work extend understanding about interaction between two transition metal oxides for the preparation of high-performance electrode materials for lithium-ion batteries by using a cheap, simple and environmentally friendly method. The possibility to adjust a properties of electrode material (rate capability, gravimetric capacity, cyclability) makes it promising for lithium-ion battery applications such as laptops, power tools, smartphones, drones, electric cars, etc.

References:

1. D. Kong et al. *J. Mater. Chem. A.* **4** p. 11800–11811 (2016)
2. Y. Yang et al. *Appl. Surf. Sci.* **463** p. 322–330 (2019)
3. K. Kaprans et al. *Solid State Ionics* **319** p. 1–6 (2018)

P77. Thermal Treatment Impact on Tungsten Boride Nanofilms

Liga Avotina[1], Annija Elizabete Goldmane[1], Edgars Vanags[2], Lada Bumbure[3]. Marina Romanova[3], Hermanis Sorokins[3], Alexei Muhin[4], Aleksandrs Zaslavskis[4], Gunta Kizane[1], Yuri Dekhtyar[3]

[1]Instiute of Chemical Physics, University of Latvia, Jelgavas St.1, Riga, Latvia
[2]Institute of Solid State Physics, University of Latvia, Kengaraga St. 8, Riga, Latvia
[3]Institute of Biomedical Engineering and Nanotechnologies, Riga Technical University, Kipsalas St. 6B, Riga, Latvia
[4]Joint-stock company "ALFA RPAR", Ropazu St. 140, Riga, Latvia
liga.avotina@lu.lv

Nuclear fusion reactors are among the perspective devices for production of energy [1]. Plasma facing materials selection and their lifetime characterization prior the implementation into the fusion devices is of great interest. Presently tungsten is the plasma facing material for the International Thermonuclear Experimental Reactor (ITER) [2]. In order to achieve better plasma performance, introduction of boron in the composition of plasma facing materials is planned [3]. There are studies on boron containing compounds [4,5], however, the information gap of thin film behaviour under thermal loads needs to be filled.

The aim of present research is to characterize the behaviour of deposited thin tungsten-boron films under thermal load. Tungsten-boron films were deposited on the Si/SiO_2 substrate by the magnetron sputtering technique with thickness of 150 nm. The synthesized films were characterized by means of exoemission and Fourier transform infrared (FTIR) spectrometry. The thermal load in a way of heating was applied up to 600°C for 6 hours. Changes in the chemical bonds were determined by means of FTIR. The obtained results of tungsten-boron films are compared with pure tungsten films. It is observed, that thermal treatment leads to formation of W-O, W=O and oxidized boron containing compounds. Exoemission of tungsten films takes place at 410°C, while films with boron addition give exoemission peak at around 485°C.

The obtained results will be applied for recommendations for lifetime predictions of boron containing tungsten films in fusion devices.

Acknowledgements: The research was supported by the ERDF project No. 1.1.1.1/20/A/109 "Planar field emission microtriode structure".

Keywords: *tungsten, boron, infrared spectrometry, thermal treatment.*

References:

1. E. R. Sadik-Zada et al. *Energy* **290** p. 129150 (2024)
2. A. Becoulet et al. *Fusion Engineering and Design* **188** p. 113424 (2023)
3. S. Sun et al. *Nuclear Materials and Energy* **31** p. 101174 (2022)
4. M. Wulmshuber et al. *International Journal of Refractory Metals and Hard Materials* **111** p. 106125 (2023)
5. Y. Hiroka et al. *Journal of Nuclear Materials* **176–177** p. 473–480 (1990)

P78. Investigation of Photoelectrochemical Systems for Production of Hydrogen and Oxidants

Milda Petruleviciene[1], Irena Savickaja[1], Jelena Kovger-Jarosevic[1], Jurga Juodkazyte[1], Arunas Ramanavicius[1,2]

[1]Center for Physical Science and Technology, Sauletekio Ave. 3, LT-10275 Vilnius, Lithuania
[2]Department of Physical Chemistry, Faculty of Chemistry, Vilnius University, Naugarduko 24, LT-03225 Vilnius, Lithuania
milda.petruleviciene@ftmc.lt

In recent years the use of renewable energy sources has increased significantly in an attempt to mitigate the global energy crisis and climate change. Photoelectrochemical (PEC) systems are among the alternative technologies to convert solar energy into valuable chemicals, such as hydrogen and oxidants. The efficiency of the PEC system strongly depends on the nature of photoanode and the composition of the electrolytes. In this study photoanodic formation of oxidants and hydrogen evolution on Pt cathode during chronoamperometric (CA) experiments.

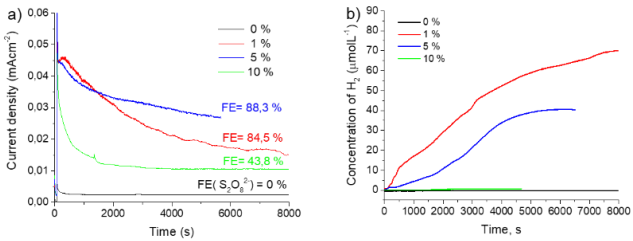

Fig. 1. Variation of photocurrent density (a) and concentration of hydrogen (b) during photoelectrolysis with W-doped $BiVO_4$ coatings in 0.1 M Na_2SO_4 at 1.2 V(Ag/AgCl); FE of PEC generation of persulfate are indicated in (a)

Fig. 1 (a) presents the results of CA experiments, where W-doped $BiVO_4$ samples were used as photoanodes in the photoelectrolysis of 0.1 M Na_2SO_4 solution. The data shows a significant improvement in photoactivity of $BiVO_4$ due to W-doping. The Faradaic Efficiency (FE) of produced reactive sulfate species (RSS) in the form of $S_2O_8^2$ for 1% and 5% W-doped coatings was observed to be ~80–88%. Results with hydrogen evolution reaction (fig. 1 (b)) followed analogous trend: the most intensive hydrogen production was observed with $BiVO_4$ coating containing 1% of W.

Acknowledgements: This project has received funding from the Research Council of Lithuania (LMTLT), agreement No S-PD-22-2.

Keywords: *bismuth vanadate, photoelectrochemical, oxidants, hydrogen.*

P79. 2D-Reduced Graphene Oxide Induced Bi-Functional Plasmonic p-n Heterostructure for Photoelectrochemical Water Splitting

Muhammad Haris[1], Klaudijus Midveris[1],Syeda Ammara Shabbir[3], Tomas Tamulevičius[1], Gvidas Klyvis[1], Mantas Mikalkevičius[1], Algirdas Lazauskas[1], Sigitas Tamulevičius[1,2]

[1]Institute of Materials Science, Kaunas University of Technology
K. Baršausko St. 59, LT-51423 Kaunas, Lithuania
[2]Department of Physics, Kaunas University of Technology, Lithuania
K. Donelaičio St. 73, LT-44249 Kaunas, Lithuania
[3]Department of Physics, Forman Christian College (A Chartered University),
Lahore 54600, Pakistan
muhammad.haris@ktu.edu

Photoelectrochemical (PEC) water splitting is considered a remarkable way for green hydrogen, which uses major chunk of solar energy and semiconductors (photocatalyst) readily available on Earth [1]. Various researches and techniques have been perceived to fabricate ideal photoelectrodes to enhance the overall PEC efficiency, and among reported research trends bifunctional heterostructures have been extensively paving the way to expedite the efficiency of both the oxygen evolution reaction (OER) and the hydrogen evolution reaction (HER) by manifesting greater Tafel slope at low over potential rate [2]. To yield the maximum PEC kinetics and tackle with less mobility of the photogenerated current, plasmonic nanoparticles can be considered because of their splendid attribute of localized surface plasmonic resonance (LSPR), which leads towards the hot electron distribution upon visible light irradiation and enhances the mobility of photogenerated electrons by exhibiting the phenomena of thermionic emission and tunnelling [1]. This study investigates indirect contact of reduced graphene oxide (RGO) induced by p-type $CuBi2O_4$ and n-type $BiVO_4$ coupled Au nanoparticles (NP) for PEC water splitting, where RGO is being used as an electron mediator to capture maximum number of electrons from one semiconductor to other, on account of their high surface to volume ratio. We demonstrate that the overall PEC efficiency of this RGO induced bifunctional plasmonic p-n heterostructure can be made more higher by coupling with Au nanoparticles (NPs).

Keywords: *OER, HER, Bi functional heterostructure, Tafel slope, thermionic emission, tunnelling.*

References:

1. S. A. Shabbir et al. S. A. *Materials Letters* **360** p. 135932 (2024)
2. Syeda Ammara Shabbir et al. *ACS Omega* **9(19)** p. 21450–21458 (2024)

P80. Environmental Impact on the Structural and Optoelectronic Behavior of Mixed Tin-Lead Perovskites

Paula Baltaševičiūtė, Rokas Gegevičius, Vidas Pakštas, Arnas Naujokaitis, Vidmantas Gulbinas, Marius Franckevičius

Center for Physical Sciences and Technology, Saulėtekio Ave. 3, LT-10257 Vilnius, Lithuania
paula.baltaseviciute@ftmc.lt

Mixed tin–lead perovskites are becoming incredibly popular because of their narrow bandgap (1.2–1.3 eV) which plays a vital role in all-perovskite tandem solar cells for achieving higher efficiencies compared to single–junction counterparts [1]. However, easy oxidation of Sn^{2+} to Sn^{4+} limits Pb-Sn perovskite stability and their performance [2]. This restricts their long-term use in all-perovskite tandem devices.

This study aims to demonstrate that mixed tin-lead perovskite structure and its optoelectronic properties respond differently to the changes in fabrication and environmental conditions. All samples were fabricated in an Argon atmosphere and subsequently measured under three different gas environments: Argon (Ar), Nitrogen (N_2), and Oxygen (O_2). The acquired absorption spectra reveal that perovskite films stored in both argon and nitrogen atmospheres remain unchanged, whereas slight variation in absorption intensity was observed after the exposing perovskite to Oxygen for 5 hours. Meanwhile, the X-ray diffraction (XRD) analysis demonstrate no structural alterations following a 24-hour exposure to a standard atmospheric environment.

Despite the structural stability of the perovskite material, the optoelectronic analysis reveals significant variations in response to environment conditions. Photoluminescence (PL) lifetime decreases by increasing oxygen concentration implying the presence of strong nonradiative channel, probably associated with energetic disorder within the material. Furthermore, transient photocurrent measurements additionally reveal that even small quantities exert a pronounced influence on the trap concentration, leading to their substantial increases as oxygen levels rises.

Acknowledgments: This research was funded by a grant (Agreement No. P-MIP-22-210) from the Research Council of Lithuania.

Keywords: *photoluminescence spectroscopy, Sn-Pb mixed perovskite, structural characterization, transient photocurrent.*

References:

1. Y. Gao et al. *Joule* **6(8)** p. 1944–1963 (2022)
2. H. Lee et al. *Nano Convergence* **10** p. 27 (2023)

P81. Comparative Analysis of Methane Pyrolysis Catalysts Supported on Alumina and Titania

Raitis Kaspars Sika[1], Ainārs Konks[1], Ansis E. Zīvers[1], Līga Grīnberga[1], Šarūnas Varnagiris[2], Marius Urbonavicius[2]

[1]Institute of Solid State Physics University of Latvia, Riga, Latvia
[2]Center for Hydrogen Energy Technologies, Lithuanian Energy Institute, Breslaujos St. 3, LT-44403 Kaunas, Lithuania

According to EU initiatives for clean energy transition such as the SDG7, novel catalysts with use in sustainable energy production will play a key role for the transition. Hydrogen is expected to compose a substantial part in our clean future, but implementation is lagging behind, partially due to high costs.

One alternative for this transition period is low-cost hydrogen production, but conventionally it brings carbon related emissions. Even though there is an alternative, pyrolysis of methane, conventional technologies involve high temperatures and pressures, which means a high energy demand. To reduce the temperature and therefore the energy demand, a catalyst must be used.

Our aim is to develop an innovative catalyst for methane pyrolysis by depositing iron with widely dispersed nickel nanoclusters on gamma alumina using the magnetron sputtering technique. Gained results, such as hydrogen yield, produced by-gases, and residual materials, will be compared with those obtained using titania as the substrate material.

The investigation of substrate materials and catalysts in combination with the analysis of produced gases enables the optimization of both the catalyst and the pyrolysis process. Samples were characterized using scanning electron microscopy, X-ray powder diffraction, and Raman spectroscopy. Information about the thermal stability of samples, decomposition kinetics, and other thermal properties was obtained through thermogravimetric analysis. Hydrogen production was measured using gas chromatography and mass spectrometry.

Keywords: *iron-nickel nanoclusters, clean energy, hydrogen, pyrolysis, nanomaterials.*

P82. Enhancing Electron Transfer Efficiency in Microbial Fuel Cells through Gold Nanoparticle Modification of *Saccharomyces cerevisiae*

Teresė Kondrotaitė, Inga Morkvėnaitė-Vilkončienė

Vilnius Gediminas Technical University
Saulėtekio Ave. 11, LT-10223 Vilnius, Lithuania
terese.kondrotaite@vilniustech.lt

Microbial Fuel Cells (MFCs) present a sustainable alternative for energy generation and wastewater treatment. However, their practical application is limited by the restricted charge transfer through cell walls and membranes. This study investigates the use of gold nanoparticles (AuNPs) to augment the conductivity of baker's yeast (*Saccharomyces cerevisiae*) cell wall in microbial fuel cells. Electrochemical evaluations revealed that yeast:AuNP-modified graphite electrodes produced a higher power density of 22.8 mW/m^2, albeit with a lower current density, compared to electrodes modified solely with yeast which produced a power density of 5.7 mW/m^2. Despite certain challenges, the findings suggest promising potential for incorporating AuNPs in MFCs to enhance biofuel cell performance. Future research should focus on refining the AuNP modification process to optimize benefits, potentially facilitating broader adoption of MFCs as sustainable energy sources.

Keywords: *Microbial Fuel Cells (MFCs), biofuel cells, gold nanoparticles (AuNPs), graphite electrodes, Baker's Yeast (Saccharomyces cerevisiae).*

P83. Concentration Quenching in Solutions of Chlorophyll Molecules

Vilius Čirgelis[1,2], Simona Streckaitė[1], Jevgenij Chmeliov[1,2], Leonas Valkūnas[1], Andrius Gelžinis[1,2]

[1]Center for Physical Sciences and Technology, Saulėtekio Ave. 3, LT-10257 Vilnius, Lithuania
[2]Vilnius University, Physics Faculty, Saulėtekio Ave. 9, LT-10222 Vilnius, Lithuania
vilius.cirgelis@ftmc.lt

Most of the organic fluorophores in low concentration solutions have photoluminescence quantum yield (PL QY) that is close to 1, meanwhile PL QY is much lower for high molecule concentrations [1]. The phenomenon in which the fluorescence QY of molecules strongly decreases with an increase in their concentration is called concentration quenching. Concentration quenching could have negative effects on system or instrument performance, so it is important to understand the underlying physical action mechanism. For organometallic compounds, such as chlorophyll (Chl), this phenomenon is particularly interesting due to its role in photosynthetic complexes. However, there is no clear model that would explain concentration quenching.

The aim of the study was to examine the concentration effects on Chl-a molecules in different polarity solvents. For this investigation, absorption and fluorescence spectra and fluorescence decay kinetics were measured. Chl-a solutions were obtained by dissolving molecules in toluene and dimethylsulfoxide (DMSO).

For Chl-a solutions in toluene, with increase of concentration, the ~730 nm fluorescence band shift to 705 nm is observed, also, the intensity of the main fluorescence band at ~670 nm decreases. For Chl-a molecules in DMSO, there is no shift for 730 nm band, however, the same decrease in intensity for 670 nm band is observed. For samples in both solvents, fluorescence decay kinetics are quenched. No quenching is observed for 0.02–1 mM concentrations, while for higher concentrations, the fluorescence lifetime is lower by 2–3 times.

Keywords: *chlorophyll a, concentration quenching.*

References:

1. B. Zhang et al. *Chemistry of Materials* **29(19)** p. 8395–8403 (2017)

P84. Synthesis of Nickel and Nitrogen-doped Biomass-based Activated Carbon Catalyst for Hydrazine Oxidation

Virginija Ulevičienė[1], Aldona Balčiūnaitė[1], Daina Upskuvienė[1], Galina Dobele[2], Aleksandrs Volperts[2], Ance Plavniece[2], Aivars Zhurinsh[2], Loreta Tamašauskaitė-Tamašiūnaitė[1], Eugenijus Norkus[1]

[1]Department of Catalysis, Center for Physical Sciences and Technology, Sauletekio Ave. 3, LT-10257 Vilnius, Lithuania
[2]Latvian State Institute of Wood Chemistry, Dzerbenes St. 27, LV-1006 Riga, Latvia
virginija.uleviciene@ftmc.lt

Biomass-derived carbons have emerged as promising potential alternatives to conventionally produced carbon-based catalysts. They hold great promise as a renewable source of sustainable carbon materials for the next generation of energy storage and conversion systems. Biomass is a hot carbon precursor in terms of its renewability, earth-abundance, environmental friendliness, low-cost, non-toxicity, sustainability, ease of production, and the variety of heteroatoms (N, P, S etc.) in its intrinsic composition. Here, we present a simple strategy for the synthesis an efficient non-noble metal-based carbon catalyst. First, a biomass-based activated carbon material (AWC) was synthesized using a birch wood as the raw material. Then, nickel and nitrogen were co-doped in one step using the reaction mixture containing Ni^{2+} ion source, AWC, and dicyandiamide (DCDA) in dimethylformamide (DMF). DMF was evaporated and the mixture was treated for 60 min at a temperature of 800ºC. Detailed physicochemical analysis of the newly prepared catalyst was carried out using ICP-OES, XRD, XPS, SEM-EDS, TEM, BET, and Raman spectroscopy. It was found that the synthesized AWC-Ni-N contained approximately 1.12 at.% of Ni and 98.88 at.% of C. The electrocatalytic activity of the AWC-Ni-N catalyst towards the electrooxidation of hydrazine (N_2H_4) was evaluated using cyclic voltammetry by recording cyclic voltammograms in 1 M KOH solution containing different concentrations of N_2H_4 in the potential range of -1.2 V to 0.2 V (vs. SCE) at an electrode potential scan rate of 50 mVs^{-1}. AWC-Ni-N exhibits excellent activity and stability for the electrooxidation of N_2H_4 and appears to be a promising anode catalyst for direct hydrazine fuel cells (DHFC).

Index of Contributors

E

F

G

H

I

J

K

L

M

N

O

P

R

S

T

U

V

W

Y

Z

ADVANCED MATERIALS AND TECHNOLOGIES
BOOK OF ABSTRACTS
OF 26th INTERNATIONAL CONFERENCE-SCHOOL

ISSN 2669-1930 (online)

Authors hold responsibility for the Journal language

SL 344. 2024-07-16. 8 printer's sheets. Order No. 129
Publisher Kaunas University of Technology, K. Donelaičio st. 73, LT-44029 Kaunas
Publishing House "Technologija", Studentų st. 54, LT-51424 Kaunas

ORGANIZERS

SPONSORS