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CHEMISTRY & CHEMICAL TECHNOLOGY CONFERENCE 2026 KAUNAS

Kaunas Ch 2026

Chemistry and Chemical Technology 2026

International Scientific Conference

May 22 2026, Kaunas, Lithuania

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Editors of a Conference Book of Abstracts

Dr. Rasa Paleckienė (Kaunas University of Technology, Lithuania)
Dr. Rasa Šlinkšienė (Kaunas University of Technology, Lithuania)

The international scientific conference **"Chemistry and Chemical Technology 2026" (CCT2026)** continues a long-standing tradition of bringing together researchers, academics, and early-career scientists working in the broad fields of chemistry and chemical technology. The 2026 edition marks the 20th conference in this series.

The conference will take place on **22 May 2026** in **Kaunas, Lithuania**, and is organized by the **Faculty of Chemical Technology of Kaunas University of Technology**, in cooperation with academic and research partners.

The 2026 edition of the conference marks **the 100th anniversary of the birth of two distinguished professors of the Faculty of Chemical Technology – Professor Romualdas Baltrušis and Professor Vaclova Zelionkaitė** – whose scientific, academic and educational contributions significantly shaped the development of chemical sciences, chemical technology and higher education in Lithuania.

CCT2026 is a one-day international forum designed to provide a high-quality platform for presenting and discussing the latest scientific results, new ideas, and technological achievements. The conference will feature **keynote lectures by internationally recognized scientists**, oral presentations in thematic sessions, and a poster session, offering opportunities for both experienced researchers and young scientists to present their work and engage in scientific exchange.

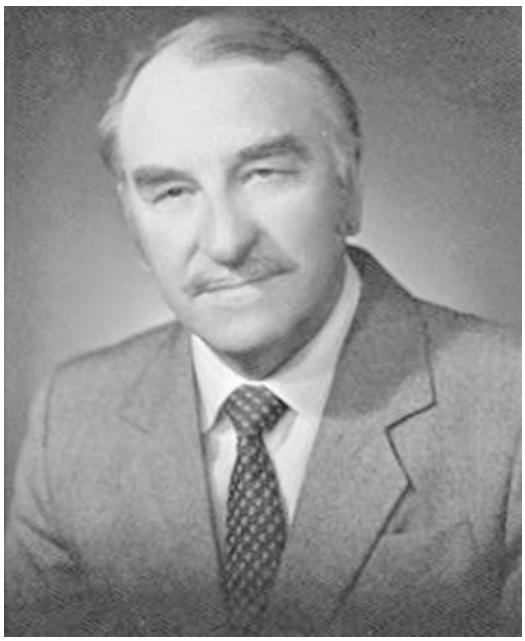
In addition, **CCT2026 will include a parallel student scientific conference**, aimed at providing undergraduate and graduate students with an opportunity to present their research results, develop scientific communication skills, and engage with the broader academic community.

The official language of the conference is **English**.

The conference topics listed below are common to all participants, including contributors to the parallel student scientific conference.

- Advanced Materials Chemistry and Functional Materials
- Chemical Engineering, Process Systems and Technology
- Sustainable Chemical and Environmental Technologies
- Bioactive Compounds, Biotechnology and Food Systems
- Applied and Medicinal Chemistry
- Electrochemistry, Energy Materials and Sustainable Energy Solutions
- Analytical Chemistry and Advanced Characterization Methods

Prof. ROMUALDAS BALTRUŠIS



On May 1 of this year, Professor Romualdas Baltrušis, a distinguished scientist and habilitated doctor, celebrates his 100th birthday. For most of this long period, Prof. R. Baltrušis devoted his work to the Kaunas Polytechnic Institute and its successor, Kaunas University of Technology.

Romualdas Baltrušis was born on May 1, 1926, in Ukmergė. After graduating from Antanas Smetona Gymnasium in Ukmergė in 1945, he studied chemistry at Kaunas University and, having graduated with honours, began his scientific career in 1950 as a postgraduate (aspirant) at the D. Mendeleev Institute of Chemical Technology in Moscow under Prof., Academician V. Radionov. From 1952, he continued his work at the Department of Organic Chemistry of the Kaunas Polytechnic Institute (KPI), where, under the guidance of Academician Antanas Purėnas, he investigated the synthesis of β-amino acids and their derivatives. As early as 1954, he defended his Candidate of Sciences (Chemistry) dissertation, “Synthesis and transformations of N-aryl β-amino acids,” and sixteen years later, in 1970, he defended his doctoral dissertation devoted to the synthesis of N-aryl, N-pyridyl, and N-quinolyl β-alanines and their transformations into pyrimidine derivatives. In 1973, he was awarded the academic title of Professor.

R. Baltrušis served as a professor for eight years. In 1980, he was elected Head of the Department of Organic Chemistry and led the department until 1990. Thereafter, until his retirement (1994), he worked as a professor in the department. Prof. R. Baltrušis was greatly appreciated by students and undoubtedly with good reason: in 1986 he won the Best Lecturer competition and delivered lecture courses in a range of subjects, including organic chemistry, bioorganic chemistry, polymer physics and chemistry, polymer chemistry, and the chemistry of wood and cellulose.

Prof. R. Baltrušis has written three textbooks, both independently and in collaboration with co-authors.: “Fundamentals of the chemistry of macromolecular compounds” (1966) and

"Organic chemistry", Parts I and II (1969/1971). For these organic chemistry textbooks, Prof. R. Baltrušis and co-authors were awarded a republican prize (1975). In 1999, Prof. R. Baltrušis prepared and published the monograph "Synthesis, transformations, and properties of N-aryl (heterocyclyl) β-alanines". Together with co-authors, he translated V. Radionov's "Practical works in organic chemistry, and edited Russian-to-Lithuanian translations of the books "Organic macromolecular compounds" and "Physical chemistry of polymers". In 1986, Professor Romualdas Baltrušis was awarded the honorary title of Distinguished Scientist of Lithuania.

Prof. R. Baltrušis, A. Machtejeva, A. Zubienė, Z. J. Beresnevičius in the laboratory of the Department of Organic Chemistry, 1971

Organic Chemistry Laboratory of Growth Regulator Synthesis: prof. R. Baltrušis, J. Bylinskaitė, V. Mickevičius, Z. J. Beresnevičius, 1986

More than 130 scientific articles published with co-authors, 49 author's certificates, nearly 40 popular-science articles, participation in 38 scientific conferences, and the supervision of 9 doctoral and 2 habilitation theses, whose graduates continue research in the synthesis of the compounds, testify to the exceptionally successful activity of this talented scientist and educator. We congratulate Professor Romualdas Baltrušis on this honourable jubilee and wish him strong health and continued success in his diverse and fruitful endeavours.

Prof. VACLOVA ZELIONKAITĖ

In 2026, we celebrate the 100th anniversary of the birth of Professor Vaclova Zelionkaitė – a distinguished Lithuanian chemist, habilitated doctor, professor, State Prize laureate, and long-standing academic of the Faculty of Chemical Technology.

Vaclova Zelionkaitė was born on 11 May 1926 in Girstupis village, Kaunas district. After graduating from Kaunas 5th Gymnasium, she entered the Faculty of Chemical Technology of Kaunas State Vytautas Magnus University in 1945 and graduated in 1950. While still a student, she began her first scientific work under the supervision of Academician Jonas Janickis.

In 1955, V. Zelionkaitė defended her dissertation and was awarded the degree of Candidate of Chemical Sciences. In 1964, she defended her Doctor of Chemical Sciences dissertation, titled *Research in the Field of Selenium Oxyacids*, which was later recognised as equivalent to a habilitated doctor degree. She became the first woman in Lithuania to be awarded the Doctor of Chemical Sciences degree. In 1968, she was awarded the academic title of Professor. Professor Zelionkaitė worked at the Department of Physical Chemistry until 1969, where she taught courses in physical and colloid chemistry, sulphuric acid technology, and fixed nitrogen technology. She supervised laboratory work, diploma projects, industrial placements, and the scientific work of postgraduate students and colleagues.

From 1969 to 1985, Prof. V. Zelionkaitė served as Head of the Department of Inorganic Chemistry and later continued her work as professor of the department. She taught courses in general and inorganic chemistry and supervised laboratory and research-based teaching activities in inorganic and analytical chemistry. Her main research field was the chemistry of sulphur, selenium, tellurium and arsenic compounds, including the formation, properties and transformations of oxyacids containing these elements. Her scientific work led to the synthesis and characterization of about 50 new inorganic compounds, some of which showed biological activity and potential for applications in conductive and semiconductive films on polymer

materials. She also led applied research contracts with industrial enterprises and research institutes in Lithuania and abroad.

V. Zelionkaitė graduated from the Faculty of Chemical Technology, 1950
(Prof. V. Zelionkaitė family archive)

Commemoration of chemists' anniversaries at the Faculty of Chemical Technology of KTU, 1996. From left: Prof. E. Pacauskas, Prof. R. Baltrušis, Prof. B. Stulpinas, Prof. V. Zelionkaitė, Prof. J. Janickis. (KTU Museum)

Prof. Zelionkaitė authored and co-authored more than 150 scientific publications and received 7 author's certificates. She made a substantial contribution to chemical education by preparing teaching and methodological publications, including *Sulphuric Acid Production* (1968), *Laboratory Works in Physicochemical Analysis*, *Lecture Notes in Inorganic Chemistry* (Part I, 1972; Part II, 1975), and *Laboratory Works in General and Inorganic Chemistry*, which was published in six editions between 1972 and 1997. In 1995, she also published the textbook *General and Inorganic Chemistry*.

Professor Vaclova Zelionkaitė passed away on 13 August 2017. Her scientific achievements, pedagogical work, and dedication to academic life remain an important part of the history of inorganic chemistry, chemical education, and the Faculty of Chemical Technology.

Invited Speakers

Assoc. Prof. Jonas Baltrušaitis

Department of Chemical and Biomolecular Engineering
Lehigh University, USA

Jonas Baltrušaitis is an Associate Professor of Chemical and Biomolecular Engineering at Lehigh University, whose work is characterized by a multidisciplinary approach to sustainable chemical engineering and molecular-level surface science. He earned his PhD in Physical Chemistry from the University of Iowa in 2007 and has authored more than 300 peer-reviewed publications. His research spans fundamental catalysis and atmospheric chemistry, as well as smart nutrient-delivery systems for sustainable agriculture. Using advanced surface-sensitive spectroscopies, he connects theoretical physical chemistry with practical engineering solutions for global challenges, including the remediation of forever chemicals and catalytic processes in fossil fuel refining.

Presentation Overview

In the realm of electrochemical CO_2 reduction, Prof. Baltrušaitis focuses on the conversion of greenhouse gases into value-added fuels and chemical feedstocks, such as formic acid, methane, and ethylene. His research is particularly distinguished by its move toward realistic industrial applications, investigating how catalysts perform under dilute flue gas conditions rather than idealized pure CO_2 streams.

By engineering specialized electrode surfaces, such as tin-decorated copper oxides, his group has achieved high Faradaic efficiency while suppressing the competing hydrogen evolution reaction. Through the integration of X-ray Photoelectron Spectroscopy and computational modelling, his work provides mechanistic insights necessary to develop a low-temperature redox cycle, ultimately supporting the transition toward a sustainable, solar-fuel-based economy.

Prof. Rasa Pauliukaitė

Department of Nanoengineering,
Center for Physical Sciences and Technology,
Lithuania

Professor Rasa Pauliukaitė is a chemist and leading Chief Researcher at the Department of Nanoengineering, where she also heads the Laboratory of Functional Nanomaterials. She obtained her PhD in Physical Sciences at the Institute of Chemistry in Vilnius in 1998 and gained postdoctoral experience in Austria, Slovenia, Switzerland, and Portugal. Her research over more than 20 years has focused on the development of materials for sensors and the optimization of their architecture to achieve improved analytical performance, including sensitivity, stability, and selectivity. She has supervised seven PhD students and has extensive experience in international collaboration with academic institutions worldwide.

Presentation Overview

Electroanalysis is a subdiscipline of electrochemistry focused on the development of novel techniques, analytical methodologies, and modified electrode systems for quantitative analysis. Recent advances have expanded the range of detectable analytes and improved the reproducibility and robustness of electrochemical sensors, making them increasingly suitable for continuous monitoring and point-of-care diagnostics.

Our research group develops electrochemical sensors for a broad range of applications, including health monitoring, plant health studies, archaeological sample investigation, and fungal detection. A central aspect of this work is the exploration and integration of advanced materials, with particular emphasis on carbon-based nanomaterials and conducting polymers, as well as electrochemical approaches for detecting both electroactive and non-electroactive species.

In this contribution, we present key aspects of the synthesis, characterisation, and application of these materials in the electrochemical sensing of diverse analytes and applications.

Prof. Maris Turks

Faculty of Natural Sciences and Technology
Riga Technical University, Latvia

Māris Turks is Professor at the Faculty of Natural Sciences and Technology, Riga Technical University, Latvia. He obtained his doctoral degree in organic chemistry from the Swiss Federal Institute of Technology in Lausanne and subsequently spent one year as a Postdoctoral Fellow at Stanford University. In 2007, he returned to Riga Technical University and started his independent academic career. He served as Director of the Institute of Technology of Organic Chemistry during period 2010-2023 and as Dean of FMSAC RTU during period 2018-2023. Since 2024, Prof. Turks is Dean of the Faculty of Natural Sciences and Technology, RTU. Since 2015, M. Turks serves as associate editor of SCI journal "Chemistry of Heterocyclic Compounds". Prof. Turks' research interests include organosilicon and organogermanium chemistry, sulfur dioxide chemistry, carbohydrate and nucleoside chemistry, functionalized heterocycles, energetic compounds, and natural triterpenoids.

Presentation Overview

The lecture will present recent advances in 1,2-metalloid shift chemistry of propargyl silanes and germanes for the stereocontrolled synthesis of allylic and heterocyclic systems. Electrophilic activation of propargyl metalloids induces vinyl cation–allyl cation rearrangements through 1,2-metalloid migration, generating reactive intermediates suitable for intermolecular and intramolecular trapping by various nucleophiles. The developed methodology enables efficient access to multifunctionalized products containing vinyl halide, vinyl silane, and heterocyclic motifs, which can be further transformed by cross-coupling and allylic substitution reactions. Mechanistic aspects of electrophile-induced rearrangements, stereocontrolled double-bond formation, and multicomponent processes involving sequential nucleophilic additions will be discussed. The presented work demonstrates the synthetic potential of metalloid migration strategies for the preparation of structurally complex organic molecules.

Assoc. Prof. František Šoukal

Faculty of Chemistry Brno
University of Technology, Czechia

František Šoukal is affiliated with the Faculty of Chemistry at Brno University of Technology in Czechia, where he has long been engaged in research in the field of inorganic materials chemistry and physics. His expertise is strongly focused on the chemistry and technology of cementitious and construction materials, particularly on the processes governing their formation, transformation, and long-term performance. His research specializes in the mineralogical and microstructural aspects of reaction processes, with particular emphasis on hydration and carbonation of cementitious and alternative binder-based secondary raw materials. His research group has recently focused on the development of ultra-high-performance concretes for ballistic protection of critical infrastructure, carbonation hardening of inorganic binders, and the development of low-emission and sustainable construction materials.

Presentation Overview

The plenary lecture focuses on reducing CO_2 emissions in the energy-intensive cement industry through the mineral carbonation of calcium silicate-based materials. It presents carbonation as an effective approach for long-term CO_2 sequestration while simultaneously improving the mechanical properties of non-cementitious materials.

The core of the presentation addresses a detailed investigation of the accelerated carbonation of γ-C_2S using isothermal calorimetry, including the development of custom high-pressure ampoules that enable measurements under elevated CO_2 pressures. The results demonstrate that carbonation is a rapid and strongly exothermic process, occurring predominantly within the first hours and leading mainly to the formation of crystalline phases such as calcite and aragonite, alongside amorphous products.

The lecture further highlights the influence of process parameters on reaction kinetics and confirms that isothermal calorimetry is a suitable method for studying carbonation under controlled conditions, with the water-to-solid ratio identified as a key factor.

Assoc. Prof. Vaidotas Kisielius,

Department of Environmental Science,
Aarhus University, Denmark

Vaidotas Kisielius works at Aarhus University, Department of Environmental Science, in the field of Environmental Chemistry & Toxicology. In collaboration with international partners, he focuses on advanced mass spectrometry methods for the analysis of trace organic compounds in complex environmental samples. His research includes high-resolution mass spectrometry, environmental chemistry, micropollutant fate, environmental metabolomics, and advanced wastewater post-treatment technologies.

Presentation Overview

Mass spectrometry imaging (MSI) is a relatively new analytical technique that allows not only identification of compounds present in a sample, but also determination of their spatial distribution. In this presentation, the capabilities of MSI to enable simultaneous detection of compounds, without the need for chemical labelling, will be introduced. The approach is applicable across environmental science, biology, biotechnology, medicine, and materials research. It can be used to illustrate the distribution of pollutants in heterogeneous environmental samples, track metabolites in biological tissues, follow pharmaceuticals within organs, and investigate additives, degradation products, and contaminants within polymers and other complex materials.

The concept will be illustrated through two selected case studies. First, MSI applied to wastewater biofilms shows that micropollutant degradation is not uniform, but occurs in localized “hotspots” within the biofilm structure. Second, an example from environmental toxicology demonstrates that MSI can map the distribution of contaminants in biological tissues, such as in the nervous system of an intact, multicellular aquatic organism.

Assoc. Prof. Eugenijus Urnėžius

Department of Chemistry and Biochemistry
University of Portland, USA

Eugenijus Urnėžius graduated from Vilnius University in 1992. He continued his studies at Case Western Reserve University (1994–1999) under the guidance of Prof. John D. Protasiewicz and, after defending his PhD thesis, joined the group of Prof. John E. Ellis at the University of Minnesota for postdoctoral training (1999–2001). He began his independent academic career at Michigan Technological University in 2001 and moved to the University of Portland in 2009, where he is currently Associate Professor in the Department of Chemistry and Biochemistry. His research focuses on electroactive organophosphorus compounds and coordination complexes supported by multidentate phosphorus/sulfur ligands.

Presentation Overview

2,5-Di(phosphino)-1,4-hydroquinones function as effective binucleating ligands towards Ni(II) centers. Their derivatives, 2,5-di(phosphoryl)-3,6-di(X)-1,4-hydroquinones (phosphoryl = -P(=O)Ph2 or -P(=O)iPr2; X = F or Cl), readily undergo double oxidative dehalogenation yielding 2,5-dihydroxy-1,4-quinones appended with two -P(=O)R2 groups. These compounds are redox-active, engage in strong hydrogen bonding with water, and display versatile coordination chemistry towards Cu(II) centers.

Replacing -P(=O)R2 groups on 2,5-dihydroxy-1,4-quinone with two phosphonato (-P(=O)(OR)2; R = Me or Et) substituents profoundly affected the solubilities of the functionalized dihydroxy quinones in both water and organic media. In addition, 1,4-hydroquinones appended with two -P(=O)R2 or -P(=O)(OR)2 groups were also found to function as single-benzene fluorophores. Spectroscopic, structural, and electrochemical properties of these compounds, as well as synthetic methods used in their preparation, will be presented and discussed.

PROGRAMME

8.00 – 9.00 Registration and Welcome Coffee (Santaka Valley)

9.00 – 9.30 Opening of the Conference (Santaka Valley)

- Opening address by the Vice-Rector for Research of Kaunas University of Technology
- Academic tributes in honour of Prof. Romualdas Baltrušis and Prof. Vaclova Zelionkaitė

9.30 – 11.00 Plenary Session – Keynote Lectures (Santaka Valley):

Session chairs: Prof. Vaida Kitrytė-Syrpa and Assoc. Prof. Vaidotas Kisielius

- Assoc. Prof. Jonas Baltrušaitis, Lehigh University (USA). Storing electron energy in high-value chemicals: from flue gas CO_2 electrochemical oxidation to formic acid co-production
- Prof. Rasa Pauliukaitė, Center for Physical Sciences and Technology (Lithuania). How could electroanalysis help improve well-being?
- Prof. Maris Turks, Riga Technical University (Latvia). 1,2-Metalloid Shift-Enabled Access to Allylic and Heterocyclic Systems from Propargyl Metalloids

11.00 – 11.30 Coffee break / Poster presentations / Exhibition by Industrial Partners (Santaka Valley)

11.30 – 13.00 Plenary Session – Keynote Lectures (Santaka Valley):

Session chairs: Prof. Vaida Kitrytė-Syrpa and Assoc. Prof. Jonas Baltrušaitis

- Assoc. Prof. Vaidotas Kisielius, Aarhus University (Denmark). Visualizing metabolism: mass spectrometric imaging of localized biotransformation in biofilms
- Assoc. Prof. František Šoukal, Brno University of Technology (Czech Republic). Mineralogical Insights into Accelerated Carbonation Products
- Assoc. Prof. Eugenijus Urnėžius, University of Portland (United States of America). Expanded roles of benzoquinonoid platform rendered by phosphine, phosphine oxide, or phosphonato appendages: binucleating ligands for Ni(II) or Cu(II) centers, water-soluble electroactive substances, and single-benzene fluorophores

13.00 – 14.00 Lunch Break / Poster presentations / Exhibition by Industrial Partners (Santaka Valley)

14.00 – 16.30 Parallel Sessions in Thematic Sections

- International Scientific Conference
  Parallel Sessions in Thematic Sections (Santaka Valley)
- Student Scientific Conference
  Oral Presentation Sessions in Thematic Sections (Faculty of Chemical Technology)

16.30 – 17.00 Coffee Break / Poster presentations / Exhibition by Industrial Partners (Santaka Valley)

17.00 – 17.30 Awards and Closing of the Conference (Santaka Valley)

Content

HOW COULD ELECTROANALYSIS HELP IMPROVE WELL-BEING?

Rasa Pauliukaite[1]*, Pamela Rivera[1], Justina Stonytė[1], Paulina Morkytė[1], Edita Voitechovič[1], Justina Gaidukevič[1], Islam Hassan[1], Kazem Karb[1], Mohamed Abdelkader[1], Vytautas Žutautas[2]

[1] Department of Nanoengineering, Center for Physical Sciences and Technology, Vilnius, Lithuania
[2] Department of Nuclear Research, Center for Physical Sciences and Technology, Vilnius, Lithuania
* *rasa.pauliukaite@ftmc.lt*

Electroanalysis is a subdiscipline of electrochemistry that focuses on the development of novel techniques, analytical methodologies, and modified electrode systems for quantitative analysis. Traditionally, electroanalysis has been employed as a rapid and sensitive approach for the determination of small electroactive molecules. The field of electroanalysis encompasses a wide range of techniques that enable the detection of larger and/or non-electroactive species, either through indirect electrochemical processes or by monitoring changes in interfacial properties, such as resistance variations in impedimetric sensors [1]. Recent methodological and technological advances have not only expanded the spectrum of detectable analytes but have also significantly enhanced the reproducibility and robustness of electrochemical sensors. As a result, electroanalytical techniques have become increasingly suitable for applications requiring continuous monitoring [2] as well as for point-of-care diagnostics.

Our research group focuses on the development of electrochemical sensors for a broad range of applications, including health monitoring, such as the detection of neurotransmitters [3-6]. A central aspect of our sensor development strategy is the exploration and integration of advanced materials, with particular emphasis on carbon-based nanomaterials [3–8] and conducting polymers [8]. Electroanalytical approaches have also been applied to the investigation of plant health, including growth monitoring by the analysis of heavy metal accumulation in Swiss chard leaves [9]. In addition, our work encompasses the investigation of archaeological samples and the detection of fungal species [10].

In this contribution, we present and discuss key aspects of the synthesis, characterisation, and application of these materials in the electrochemical sensing of diverse analytes and applications.

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1,2-METALLOID SHIFT-ENABLED ACCESS TO ALLYLIC AND HETEROCYCLIC SYSTEMS FROM PROPARGYL METALLOIDS

Māris Turks*, Artjoms Ubaidullajevs, Rasma Kroņkalne, Rūdolfs Beļaunieks, Sandra Turka, Rihards Lācis, Krišjānis Gercāns, Raimonds Rogaļevs, Mikus Puriņš, Armands Sebris

Institute of Chemistry and Chemical Technology, Faculty of Natural Sciences and Technology, Riga Technical University, Latvia
* *maris.turks@rtu.lv*

1,3-Difunctionalizations are far less common in organic synthesis than their 1,2- and 1,4-counterparts. Propargyl silanes and germanes can act as precursors of 1,3-dipols, if their electrophilic activation is followed by 1,2-metaloid shift, which generates carbocation or its equivalent [1,2]. The latter undergoes a proton loss to provide a stable final product if no nucleophile is present in the reaction mixture [3].

Herein, we report a substantial development of this approach, which profits from the vinyl cation - allyl cation rearrangement via 1,2-metaloid shift (Fig 1). Thus, propargyl silanes and germanes of type 1 react either with proton, $PhSe^+$, halogen electrophiles or *in situ* generated organocopper(III) species forming intermediates of type 3.

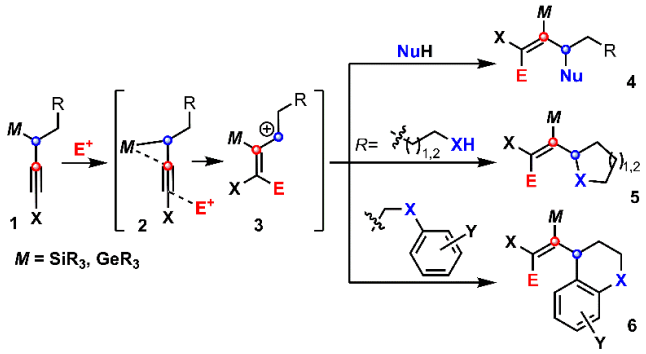

Fig. 1. Electrophile-induced 1,2-migration of propargyl metalloids with subsequent nucleophilic quenching.

The electrophile approaches antiperiplanar to the trajectory of metalloid migration, enabling stereocontrolled double-bond formation. In the next step various *N*-, *O*-, *S*- and *C*-nucleophiles are added either intramolecularly or intermolecularly [4–7]. Subsequent reactions, such as C-C cross-coupling reactions involving vinyl halide or vinyl silane moieties and allylic substitution, have been demonstrated for further modification of products 4-6. We have also explored a multicomponent Ritter-type process, which after nitrile addition terminates with the attack of second nucleophile.

Acknowledgements. This work was supported by the Latvian Council of Science Grant LZP-2023/1-0576.

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INVESTIGATION OF PHENANTHROIMIDAZOLE–QUINOXALINE DERIVATIVES AS BLUE EMITTERS EXPLOITING HYBRIDIZED LOCAL AND CHARGE TRANSFER STATES

Mohamed Abdella[1]*, Melika Ghasemi[1], Jurate Simokaitiene[1], Dmytro Volyniuk[1], Aivars Vembris[2], Juozas Vidas Grazulevicius[1]

[1] Department of Polymer Chemistry and Technology, Kaunas University of Technology, Kaunas, Lithuania
[2-]Institute of Solid State Physics of University of Latvia, Riga, Latvia
** mohamed.abdella@ktu.edu*

High contrast ratios, broad viewing angles, flexibility, and energy economy are just a few of the many advantages of organic light-emitting diodes (OLEDs), which have attracted a great deal of interest from academics and industry and evolved significantly in recent decades [1]. Blue light emitters are a critical component for OLED displays and lighting technologies; however, their development remains a significant challenge due to inherently wide energy gaps and the difficulty of achieving balanced charge carrier injection and stability [2].

Rational design of D–A type molecules with emission from the locally excited and charge transfer states and high fluorescence quantum yields PLQY in solid state serve as a great choice for blue electroluminescent materials [2, 3]. In this work we explored the development of new blue emitters i.e. derivatives of phenanthroimidazole and quinoxaline to exploit emission from hybridized local and charge transfer (HLCT) states. By incorporating quinoxaline-based acceptors within a donor-acceptor-donor (D–A–D) molecular architecture, such materials can effectively harness triplet excitons [3].

In this work, we explore the synthesis, photophysical properties, and performance in OLEDs device evaluation of two phenanthroimidazole and quinoxaline derivatives as D–A–D emitters. A couple of blue isomeric emitters were prepared by phenanthroimidazole disubstitution at the different positions of the quinoxaline acceptor. Both the synthesized compounds demonstrated HLCT emission, nanosecond-scale short PL lifetimes and decent PLQY, with values of 18% and 21% in the solid state and of 64% and 53% in the toluene solution, respectively. These results enabled the use of these new compounds as blue electroluminescent materials for OLEDs.

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BALANCED CHARGE TRANSPORT AND EFFICIENT TADF IN A CARBAZOLE–TRIAZINE HOST FOR HIGH-PERFORMANCE WHITE OLEDS

Melika Ghasemi[1]*, Joseph Cameron[2], Mariia Stanitska[1, 4], Ugnė Seibutytė[1], Dmytro Volyniuk[1], Peter J. Skabara[2], Juozas V. Gražulevičius[1], Gjergji Sini[3]

[1] Department of Polymer Chemistry and Technology, Kaunas University of Technology, Kaunas, Lithuania,
[2] School of Chemistry, University of Glasgow, Glasgow, United Kingdom,
[3] Laboratoire de Physicochimie des Polymères et des Interfaces, CY Paris Cergy Université, France,
[4] Centre for Physical Sciences and Technology, Sauletekio Ave. 3, Vilnius LT-10257, Lithuania
** melika.ghasemi@ktu.edu*

Since the first demonstration of organic light-emitting diodes (OLEDs) in 1987, molecular design has played a central role in advancing the performance of both host and emitter materials [1]. Thermally activated delayed fluorescence (TADF) materials with donor–acceptor architectures have attracted significant attention due to their ability to harvest triplet excitons efficiently via reverse intersystem crossing [2, 3]. Recently, the development of white OLEDs (WOLEDs) based entirely on organic materials has become a major research focus. One effective strategy to achieve white emission is the controlled combination of blue and orange emitters in an appropriate ratio, yielding Commission Internationale de l'Éclairage (CIE) coordinates close to (0.33, 0.33) [4, 5].

In this work, we report a newly synthesized phenothiazine-based compound exhibiting strong orange emission, a high photoluminescence quantum yield, a small singlet–triplet energy gap, and balanced bipolar charge transport. These properties make the material a highly suitable orange TADF emitter. In addition, we present the characterization of a novel carbazole–triazine derivative that functions as an ultrafast green TADF material, featuring an average delayed fluorescence lifetime of 101 ns, which enables rapid triplet exciton utilization. The compound also demonstrates excellent thermal stability, high triplet energy, and balanced hole and electron transport, making it a promising host material for WOLED applications [6].

By combining this host with the orange TADF emitter and a multi-resonance blue emitter, efficient white electroluminescence was achieved. The resulting WOLEDs exhibited external quantum efficiencies in the range of 11–20% and CIE coordinates of (0.35, 0.31), which are close to ideal white light. These results highlight the effectiveness of rational molecular design in achieving efficient and color-balanced WOLEDs.

Acknowledgements. This project has received funding from the Research Council of Lithuania (LMTLT), project COLED, agreement No S-MIP-24-2.

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WHITE ORGANIC LIGHT EMITTING DIODES ENABLED BY FLUORENE-BASED ASYMMETRIC THIAZOLOTHIAZOLE EMITTERS

Khushdeep Kaur[1]*, Khrystyna Ivaniuk[2], Oleksandr Bezvikonnyi[1], Asta Dabuliene[1], Juozas Vidas Grazulevicius[1]

[1]Department of Polymer Chemistry and Technology, Faculty of Chemical Technology, Kaunas University of Technology, Kaunas, Lithuania,
[2] Department of Electronic Engineering, Institute of Information and Communication Technologies and Electronic Engineering, Lviv Polytechnic National University, Lviv, Ukraine.
** khushdeep.kaur@ktu.edu*

Efficient white emission is crucial for next-generation lighting and display technologies, demanding materials that combine high color purity with operational stability [1]. Thiazolo[5,4-d]thiazole (TT), a planar and electron-deficient heterocycle, has been extensively explored in sensing applications but remains underutilized in optoelectronic systems; moreover, commonly employed symmetric derivatives suffer from aggregation-caused quenching due to strong π-π interactions [2–6]. Herein, we report fluorene-based asymmetric TT emitters (Fig. 1) with a Donor-π-Acceptor-π-Donor' architecture, enabling controlled conformational twisting and reduced intermolecular coupling.

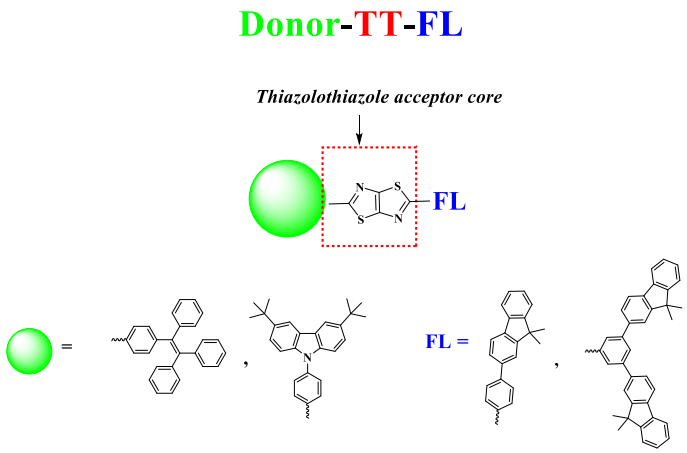

Fig. 1. Design strategy of fluorene-based asymmetric TT derivatives

These materials exhibit aggregation-induced emission enhancement, achieving photoluminescence quantum yields up to 21% in neat films and 95% in doped systems. OLED devices deliver external quantum efficiencies up to 6%, demonstrating promise for hyperluminescence and white OLED applications.

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PHOSPHOLIPID BILAYERS ON SILICON AS A PLATFORM FOR STUDYING PORE-FORMING TOXINS

Kajus Momgaudis*, Aušra Valiūnienė

Faculty of Chemistry and Geosciences, Department of Physical Chemistry, Vilnius University, Vilnius, Lithuania
** kajus.momgaudis@chgf.stud.vu.lt*

Research on phospholipid membranes remains a large focus point for improving understanding of biological processes. The phospholipid bilayer handles several critical cellular functions, including selective transport and protection against external threats. Within this framework, pore-forming toxins are of particular interest, because they directly disrupt membrane integrity and provide model systems for investigating membrane permeation mechanisms [1] relevant for pathological and antimicrobial investigations. Model phospholipid membranes have been extensively studied on functionalized metal [2,3] and metal oxide [4] surfaces. Silicon provides an attractive alternative substrate due to its well-defined surface chemistry, structural stability, and tunable electrochemical properties. Its compatibility with controlled functionalization and semiconductor-based analytical methods enables systematic investigation of interfacial phenomena at lipid membrane-semiconductor interfaces.

The objective of this study was to form and characterize bilayer lipid membranes (BLMs) composed of 1,2-dioleoyl-sn-glycero-3-phosphocholine (DOPC) on oxidized n-type silicon surfaces functionalized with an octadecyltrichlorosilane (OTS) self-assembled monolayer (SAM), and to investigate the concentration-dependent interaction of the pore-forming peptide melittin with these membranes.

Surface functionalization and membrane formation were characterized using contact angle (CA) measurements and electrochemical impedance spectroscopy (EIS). These methods were used to verify each modification step and to monitor changes in wettability, resistance, and capacitance. Melittin activity was then evaluated by exposing the BLMs to progressively increasing peptide concentrations and assessing the resulting membrane disruption.

Melittin-induced defect formation resulted in decreased membrane resistance and changes in capacitance, indicating increased ionic permeability, with a clear concentration-dependent relationship observed between melittin exposure and the extent of membrane disruption.

These results reveal that oxidized n-type silicon modified with OTS SAM provides a stable and reproducible platform for electrochemical investigation of lipid membranes. Enabling sensitive detection of melittin-induced membrane damage and offers a promising basis for semiconductor based membrane sensing platforms.

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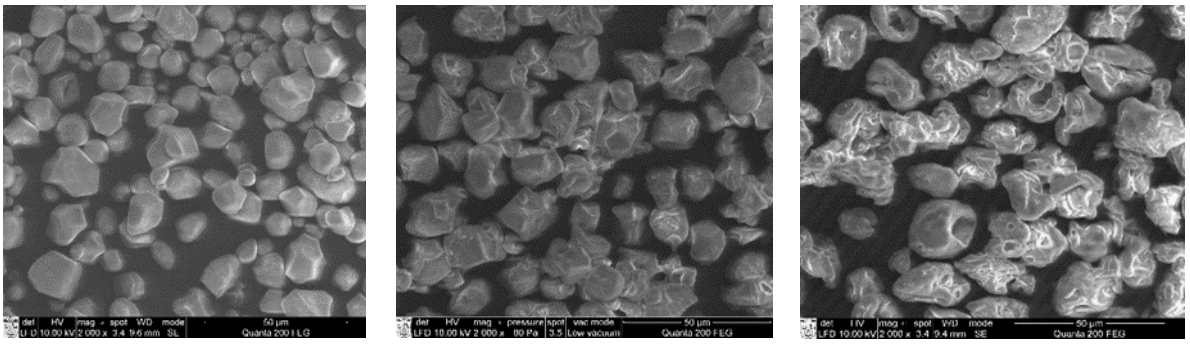
SYNTHESIS OPTIMIZATION AND FUNCTIONAL CHARACTERIZATION OF DODECENYL SUCCINIC ANHYDRIDE- AND ACETIC ANHYDRIDE-MODIFIED CORN STARCH

Muhammad Nasif[1]*, Ayodeji Amobonye[1], Joana Bendoraitiene[1], Laura Peciulyte[1], Remo Merijs Meri[2], Shu-Kai Yeh[3], Ramune Rutkaite[1]

[1] Department of Polymer Chemistry and Technology, Kaunas University of Technology, Lithuania
[2] Institute of Chemistry and Chemical Technology, Riga Technical University, Latvia
[3]Department of Materials Science and Engineering, National Taiwan University of Science and Technology, Taiwan
** muhammad.nasif@ktu.edu*

For the replacement of conventional plastics, the bioplastics based on renewable biopolymers such as natural polysaccharides are receiving increasing attention. In order to impart thermoplastic properties to polysaccharides such as starch chemical is an effective strategy to overcome the limitations of native starch.

In this study, corn starch was first modified with dodecenyl succinic anhydride (DDSA) at two substitution levels (DDSA0.025 and DDSA0.072), followed by acetylation reaction using acetic anhydride (Ac), which was optimized using central composite design. The optimized acetylation conditions yielded dual-modified starches with high degree of acetylation (Ac2.4). Structural characterization by FTIR confirmed the introduction of ester groups, while XRD analysis indicated a partial shift toward amorphous structure correlated with the degree of acetylation. Scanning electron microscopy (SEM) analysis revealed that DDSA modification helped to retain the starch granule morphology during acetylation, conferring structural resilience (Fig. 1). Thermal analyses showed that double-modified starches exhibited improved thermal stability compared to native and succinylated starches, and DSC revealed that glass transition temperature was dependent on both DDSA and acetyl group substitution. These findings demonstrate that dual dodecenyl succinic anhydride–acetic anhydride modification allows tuning of thermal and structural properties, offering potential for tailored thermoplastic applications such as biodegradable packaging materials.



a b c

Fig. 1. SEM images of St-DDSA0.025 (a), St-DDSA0.025-Ac0.53 (b), and St-DDSA0.025-Ac2.4 (c)

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ARCHITECTURE-SENSITIVE PROFILING OF FC RECEPTOR CD64 INTERACTION WITH VARIOUS IMMUNE COMPLEXES USING QCM-D AND SPECTROSCOPIC ELLIPSOMETRY

Miglė Stančiauskaitė[1]*, Asta Lučiūnaitė[2], Kristina Mašalaitė[2], Ieva Plikusienė[1]

[1] Vilnius University faculty of Chemistry and Geosciences, Vilnius, Lithuania
[2] Life Sciences Center, Vilnius, Lithuania
* *migle.stanciauskaite@chgf.stud.vu.lt*

FcγRI (CD64) is a high-affinity IgG Fc receptor on immune cells that recognizes antibody immune complexes (ICs) and helps drive their uptake and immune signaling. To quantify how IC format affects CD64 engagement under controlled conditions, CD64 was immobilized as a receptor layer and analyzed by complementary label-free methods. QCM-D reports hydrated mass and viscoelasticity, while spectroscopic ellipsometry (SE) provides dry mass and optical thickness, enabling separation of binding kinetics from hydration and architecture-related effects. Two IC formats were compared on immobilized CD64 (Fig. 1). Nb/S complexes (Fc-fusion nanobodies with SARS-CoV-2 spike) benchmarked against CR3022 IgG, and WU polyomavirus VLP/IgG complexes formed with mouse IgG1 or IgG2a. Nb/S and WU VLP/IgG2a IC interactions with CD64 resulted in K_D in the nanomolar range, with Sb15/S binding strongest and comparable to IgGCR3022/S.

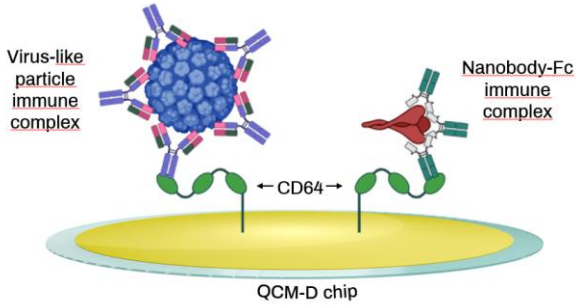

Fig. 1. Schematic of the CD64-functionalized QCM-D sensor used to compare binding of two IC formats. WU VLP/IgG (left) and Nb/S protein (right)

Optical modeling indicated a ~3.3 nm CD64 layer and thinner films for Nb/S (~18-22 nm) than for IgGCR3022/S (~30 nm), while spike alone showed negligible CD64 binding. Applying the same workflow to WU VLP/IgG revealed markedly higher hydration. VLP/IgG2a produced QCM-D frequency/dissipation responses comparable to Nb/S and a similar optical thickness (~36-38 nm), yet an ~3× higher hydrated mass. IgG1 and IgG2a ICs differed in kinetics and bound mass, consistent with subclass-dependent Fc presentation and hydration in particulate ICs.

Overall, combined QCM-D/SE analysis complements live-cell assays by isolating receptor-IC interactions in a controlled geometry while retaining sensitivity to the structural features that ultimately govern FcγRI engagement.

GNAPHALIUM ULIGINOSUM L.: OPTIMIZATION OF PRESSURIZED LIQUID EXTRACTION FOR THE PRODUCTION OF ANTIOXIDANT-RICH FRACTIONS WITH ENZYME INHIBITORY POTENTIAL

Marius Užupis[1]*, Michail Syrpas[1], Joanna Topolska[2], Małgorzata Starowicz[2], Petras Rimantas Venskutonis[1], Vaida Kitrytė-Syrpa[1]

[1] Department of Food Science and Technology, Kaunas University of Technology, Kaunas, Lithuania
[2] Department of Chemistry and Biodynamics of Food, Institute of Animal Reproduction and Food Research, Polish Academy of Sciences, Olsztyn, Poland
* *marius.uzupis@ktu.edu*

Gnaphalium uliginosum L., a traditional medicinal species belonging to the *Asteraceae* family, is known to contain bioactive compounds such as caffeoylquinic acids and flavonoids. Despite its phytochemical potential, optimal extraction conditions for obtaining bioactive fractions and for evaluating their enzyme-inhibitory properties remain insufficiently explored.

The present study aimed to optimize pressurized liquid extraction (PLE) using hydroethanolic solvent systems (PLE-EtOH/H_2O) to enhance extraction efficiency and recover fractions rich in antioxidant compounds, while also assessing their enzyme inhibitory activity. A central composite design coupled with response surface methodology was employed to investigate the influence of three independent variables: temperature (40–100 °C), extraction time (15–45 min), and ethanol concentration (20–80% v/v) on five response parameters. The optimized PLE conditions yielded extracts ranging from 20.3 to 31.3 g/100 g of plant material, exceeding those obtained via conventional ethanolic Soxhlet extraction. Additionally, the extracts exhibited elevated total phenolic content (64.9–104.6 mg GAE/g extract) and enhanced antioxidant capacity (473.0–664.0 mg TE/g extract) within a substantially reduced extraction time. The optimized extract demonstrated strong superoxide radical scavenging activity in the PCL assay (351.8 mg TE/g extract) and notable *in vitro* photoprotective properties, with SPF values increasing from 8 to approximately 50 over a concentration range of 0.1–1.0 mg/mL. Furthermore, the extract exhibited pronounced antioxidant performance in emulsion systems, as evaluated by Oxipres, indicating effective inhibition of lipid oxidation under accelerated conditions.

Further bioactivity evaluation revealed pronounced antiglycation effects and inhibitory activity against α-amylase, α-glucosidase, and pancreatic lipase, as well as moderate inhibition of angiotensin-converting enzyme (ACE), suggesting potential relevance to anti-inflammatory processes and healthy aging. Phenolic acids and flavonoids identified through HPLC–MS/MS analysis are likely responsible for the observed antioxidant and anti-inflammatory activities, supporting their applicability in functional food development.

In summary, this study presents an effective strategy for producing high-value bioactive fractions from *G. uliginosum*, highlighting its potential for use in nutraceutical and pharmaceutical applications.

ELECTROSPUN PCL NANOFIBRES FOR LOCALIZED DELIVERY OF AN ANTIMETABOLITE DRUG

Povilas Viltrakis*, Tadas Prasauskas, Edvinas Krugly

Kaunas University of Technology, Kaunas, Lithuania
** povilas.viltrakis@ktu.lt*

Electrospinning is an innovative and rapidly developing technique to produce nanofibrous materials. Nanofibres exhibit enhanced encapsulation efficiency and the potential for the simultaneous delivery of multiple therapeutic agents [1]. These properties have led to growing interest in biomedical applications, particularly drug delivery. Poly(ε-caprolactone) (PCL) is widely used in biomedicine due to its biocompatibility and biodegradability [2]. One of the commonly used chemotherapeutic agents for cancer treatment is 5-fluorouracil (5-FU), a pyrimidine analogue that inhibits tumour cell proliferation [3]. The aim of this study is to encapsulate 5-FU within electrospun PCL fibres and evaluate the drug release behaviour.

Electrospinning was used to fabricate PCL-based fibrous structures containing 5-FU. PCL was dissolved in an appropriate solvent system prior to electrospinning. By varying electrospinning parameters, including applied voltage (10–16kV), polymer concentration (13–25% (w/v) PCL), solution flow rate (0,2–2ml/h), as well as utilizing different fabrication approaches, fibres with distinct morphologies (uniform, porous, and coaxial) were developed. Fibre morphology was analysed using scanning electron microscopy (SEM) and transmission electron microscopy (TEM), and drug release kinetics were evaluated using high-performance liquid chromatography (HPLC).

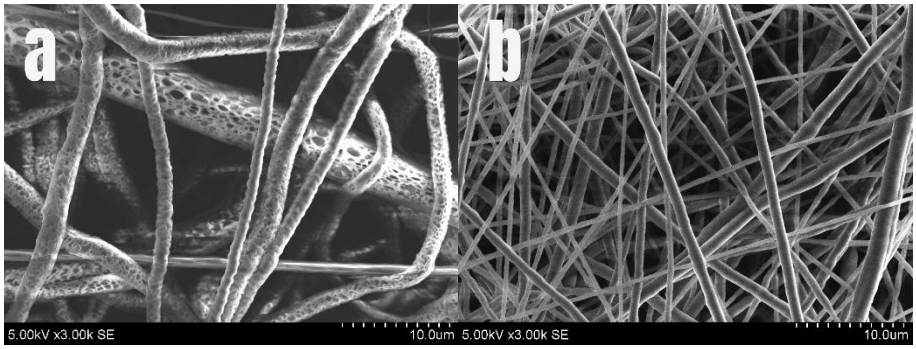

Fig. 1. SEM images of electrospun fibrous matrices (a) porous fibers; (b) uniform fibers

The results demonstrated that fibre morphology significantly influenced drug release behaviour. The obtained fibre diameters ranged from approximately 100 nm to 2 µm. Porous fibres exhibited the fastest release (up to 5 min), while uniform fibres showed a slower release profile (2–4 h), and coaxial fibres demonstrated the most sustained release (1–5 days). Coaxial fibres exhibited an initial burst release, followed by a prolonged and more controlled release phase.

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EFFECT OF DIMETHYL SULFOXIDE ON METALS IN THE PROCESS OF RECOVERING MATERIALS FROM WASTE PRINTED CIRCUIT BOARDS.

Gintaras Denafas[1, 2]*, Egidijus Griškonis[1], Gytis Miliauskas[1], Gvidas Jokubauskas[1], Remigijus Ivanauskas[1], Vidas Makarevičius[2], Arūnas Baltušnikas[2], Inna Pitak[2]

[1] Kaunas University of Technology, Kaunas, Lithuania
[2] Lithuanian Energy Institute, Kaunas, Lithuania
* *gintaras.denafas@ktu.lt*

Printed circuit boards (PCBs) are an essential component of electrical and electronic equipment (EEE); therefore, their recycling has become an important part of the overall management of waste electrical and electronic equipment (WEEE). PCBs can be considered multilayer composites consisting primarily of two or more conductive copper foil layers separated by insulating layers, typically composed of glass fiber fabric impregnated with brominated epoxy resin. PCBs also contain other critical metals, including precious and rare metals.

Delamination of the conductive and insulating PCB layers and partial dissolution of the resin represent the initial stage of waste printed circuit board (WPCB) treatment, enabling the subsequent efficient recovery of critical metals by hydrometallurgical processes. For resin dissolution, dimethyl sulfoxide (DMSO) — a solvent of relatively low toxicity and comparatively high boiling point — can be successfully applied alongside other solvents. Its effectiveness increases at elevated temperatures (up to approximately 180 °C). However, during its application, oxidation of metal surfaces (primarily copper) has been observed. This phenomenon is caused by partial thermal decomposition of DMSO, leading to the formation of sulfur-containing compounds with oxidizing properties.

Our experimental results show that during resin dissolution from shredded WPCBs, relatively significant amounts of metals — such as copper, iron, and nickel — are released into the DMSO solution. In addition, a relatively fragile surface layer consisting of copper oxide and copper sulfide forms on metallic copper particles.

The interaction between metals and DMSO is also important from an engineering perspective, as it limits the applicability of metallic reactor vessels and mechanical stirrers in the delamination process. Even when stainless steel reactors are used, the release of iron, chromium, and nickel into the solution has been observed.

Acknowledgements. This work was supported by Lithuanian Research Council in the framework of scientific projects “Materials Recovering from Multilayer Composite Waste by Simultaneous Delamination and Leaching: Theory, Technology and Circularity“ (SIMULIARITY), „Delamination of Multi-layer Electronic Waste and Recovery of Valuable Materials: Technological Device Prototype and Process Products (AMIGOS), Commercialization of a Universal Raw Material Recovery Reactor (UZARK)

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EFFECT OF WATER MATRIX SOURCE ON ELECTROCOAGULATION PERFORMANCE AT LABORATORY AND PILOT SCALES

Paulina Družaitė*, Dalia Jankūnaitė, Inga Urniežaitė

Department of Environmental Technology, Kaunas University of Technology, Kaunas, Lithuania
** paulina.druzaite@ktu.edu*

Complex water matrices, such as industrial wastewater and landfill leachate, exhibit highly variable properties and compositions, posing significant challenges to treatment and increasing the demand for efficient and sustainable technologies [1,2]. Among the available technologies, electrocoagulation (EC) has emerged as a well-established method due to its simple design and high efficiency in removing a broad range of contaminants [3]. However, most EC studies focus on a single wastewater type, limiting the understanding of how matrix source and composition influences treatment efficiency and energy consumption. This study evaluated the influence of wastewater type and matrix composition on the treatment efficiency, electrode selection, and energy consumption at laboratory and pilot scales.

Experiments were conducted using real water matrices with different characteristics, including landfill leachate (matrix 1 in Fig. 1), industrial wastewater from food sector (matrices 2,3 and 5 in Fig. 1), and mechanically biologically treated (MBT) waste leachate (matrix 4 in Fig. 1). Laboratory scale tests were performed in a 0.75 L reactor using Fe and Al electrodes at applied currents of 1–2 A, while pilot scale experiments (3.5 L) were carried out at 2 A.

The results showed that the water matrix composition plays a key role in treatment performance. Significant differences in TOC removal and changes in UV absorbance were observed under identical EC operational conditions. Electrode performance (Fe vs. Al) was dependent on the matrix type, and multivariate analysis confirmed the dominant effect of the matrix and its interactions with operational parameters.

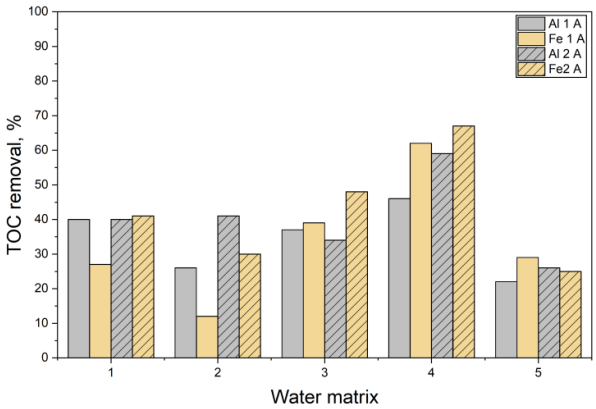

Fig. 1. Effect of water matrix source, electrode material, and current intensity on TOC removal

Scale-up results indicated that the trends observed in laboratory were not always directly transferable to pilot scale.

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APPLICATION OF MODIFIED GO ADSORBENTS FOR REMOVAL OF POLYETHYLENE NANOPLASTICS FROM FRESH WATER

Mahrosh Javed[1]*, Galina Lujanienė[1], Sergej Šemčuk[1], Vidas Pakštas[2], Aušra Selskienė[2], Martynas Talaikis[3], Audrius Drabavičius[2]

[1] Department of Environmental Research, State Research Institute Center for Physical Sciences and Technology, Vilnius, Lithuania
[2] Department of Characterization of Materials Structure, State Research Institute Center for Physical Sciences and Technology, Vilnius, Lithuania
[3]Department of Organic Chemistry, State Research Institute Center for Physical Sciences and Technology, Vilnius, Lithuania
** mahrosh.javed@ftmc.lt*

Water is essential for life on Earth. Since ancient times, civilizations have developed various techniques to purify water to ensure its safety for consumption and daily use. Over time, urbanization and industrialization have seriously contaminated air, soil, and water with substances such as heavy metals and organic pollutants. The expansion of the plastic industry and widespread improper disposal of used plastics have led to the extensive spread of microplastics (<5 mm–1 µm) and nanoplastics (<1 µm–100 nm), posing a threat to aquatic ecosystems and human health[1]. Nanoplastics (NPs) are an increasing environmental concern due to their persistence, high mobility, and potential hazards to human health and aquatic ecosystems [2]. Many techniques, including filtration, precipitation, magnetic separation, coagulation, flocculation, and adsorption, have been used to purify polluted water. Among these, adsorption has proved cost-effective and enables rapid separation. In this study, three different adsorbents – graphene oxide (GO)–chitosan and GO–microcrystalline cellulose (MCC, 50 µm and 90 µm)—were synthesized through chemical crosslinking to create sustainable polysaccharide-based composites. The novelty of this work lies in the first-time application of all these materials to the production of polyethylene (PE) nanoparticles by nanoprecipitation, as well as in the investigation of the effects of different particle sizes of the same adsorbents and different types of adsorbents. To analyze adsorption behavior in terms of morphology, chemical structure, surface chemistry, and particle crystallinity, the prepared adsorbents were characterized using scanning electron microscopy, Fourier transform infrared spectroscopy, point of zero charge, and X-ray diffraction. After adsorption, the results showed that GO–CS had the highest adsorption capacity at 50.25 mg/g, while GO–MCC–50 µm had 38.31 mg/g and GO–MCC–90 µm had 27.02 mg/g. The difference in adsorption capacity between graphene oxide–MCC (50 µm) and graphene oxide–MCC (90 µm) composites indicates that smaller adsorbent particle size significantly enhances adsorption capacity. The improved performance is attributed to stronger interaction sites, hydrophobic interactions, π–π stacking, and a greater abundance of functional groups. These findings highlight the potential of GO-functionalized biopolymer composites as sustainable and efficient adsorbents for nanoplastic removal from aqueous environments.

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INFLUENCE OF TIO_2 CRYSTALLINITY ON THE FORMATION OF $CA_XTIO_YH_2O_Z$ COMPOUNDS DURING HYDROTHERMAL SYNTHESIS AND THEIR THERMAL STABILITY

Ričardas Kleinauskas*, Anatolijus Eisinas, Jolanta Donėlienė

Kaunas University of Technology, Kaunas, Lithuania
** ricardas.kleinauskas@ktu.lt*

$CaTiO_3$-based materials are characterized by their high chemical and thermal stability, and capacity for ion exchange reactions which expands their application in photocatalysis [1], nuclear waste treatment [2] and thermoelectrical processes [3]. An increasing number of research groups are focusing on optimizing the production of $CaTiO_3$ by modifying raw materials and synthesis techniques. This work aims to investigate the influence of TiO_2 crystallinity on the formation of $Ca_xTiO_yH_2O_z$ compounds during hydrothermal treatment and their thermal stability.

In this work, amorphous TiO_2 was prepared in accordance with our earlier experiments [4]. 4 mixtures were prepared by thermally processing amorphous TiO_2 at 25, 130, 330 and 530 °C and mixing it with CaO in a molar ratio of 1. Hydrothermal treatment was performed in an autoclave (*Parr Instruments*, Germany) under saturated steam pressure of 15 bar at 200 °C for 1–96 hours. The samples were filtered, dried, sieved (<80 μm) and thermally processed at 900 °C for 1 hour in an air atmosphere. Synthesis products were characterized by XRD, FT-IR and STA instrumental methods.

XRD results indicated that, after 1 hour of hydrothermal treatment, only the $CaCO_3$ crystalline phase was present in the mixtures with amorphous TiO_2 (25, 130 °C). Additional high diffraction peaks attributed to $CaTiO_3$ were identified in the mixtures with semi-crystalline TiO_2 (330 °C). In comparison, $CaTiO_3$ crystallinity was slightly lower in the sample with fully-crystalline TiO_2 (530 °C). It was determined that increasing hydrothermal treatment to 24–96 hours had no impact on the formation of $CaTiO_3$, as its diffraction maximum intensity remained relatively similar throughout the treatment. However, extending the synthesis duration above 4 hours enhanced the formation and subsequent crystallization of kassite ($CaTi_2O_4(OH)_2$) in mixtures with amorphous TiO_2 (25, 130 °C).

To evaluate the composition of the products formed during heat treatment, the synthetic samples were calcined at 900 °C for 1 hour. It was determined that, during calcination, the synthetic amorphous compounds in the mixtures with amorphous TiO_2 (25, 130 °C) completely decomposed, forming crystalline $CaTiO_3$. $CaTiO_3$ crystallinity declined with increasing TiO_2 crystallinity (330, 530 °C). Additionally, the characteristic diffraction peaks of anatase, rutile and portlandite were detected in the XRD patterns under all experimental conditions.

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CYTOTOXICITY OF COMBUSTION-DERIVED AEROSOLS FROM LOW-SMOKE SOLID FUELS USING A NOVEL "CELLS-ON-PARTICLES" PLATFORM

Gailė Pocevičiūtė[1]*, Violeta Kaunelienė[1], Darius Čiužas[1],
Edvardas Bagdonas[2], Dainius Martuzevičius[1]

[1] Department of Environmental Technology, Kaunas University of Technology, Kaunas, Lithuania
[2] Department of Regenerative Medicine, Centre for Innovative Medicine, Vilnius, Lithuania
* *gaile.poceviciute@ktu.lt*

Combustion of solid fuels is still widely used for heating, especially in colder seasons, and significantly contributes to indoor and outdoor air pollution. It emits a complex mix of pollutants, which can cause oxidative stress, inflammation, and respiratory diseases [1]. This study aims to evaluate the cytotoxic effects of combustion-derived aerosols from different solid fuel types. The fuels were burned in a stove, and particulate matter was collected using an integrated "Cells-on-Particles" platform, enabling simultaneous particle collection and cytotoxicity assessment [2-3].

The results show that BEAS-2B cell viability depended on the type of fuel (Fig. 1). The strongest cytotoxic effects were observed for particles rich in black carbon, indicating an influence of freshly emitted soot. In contrast, particles containing higher fractions of inorganic compounds were associated with higher cell viability, suggesting lower reactivity. Biomass-derived emissions showed variable effects, with reduced viability under incomplete combustion and lower effects under more efficient combustion.

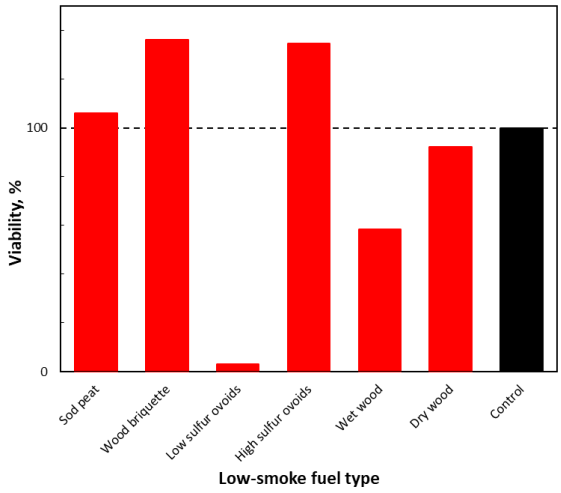

Fig. 1. Viability of BEAS-2B cells after 24 h exposure to six different low-smoke fuel aerosols

These results indicate that both the source of pollutants and combustion conditions are important factors in determining the biological effects of particulate matter generated during combustion.

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FUNCTIONAL FERRITE NANOMATERIALS: FROM DESIGN TO APPLICATIONS

Simonas Ramanavicius*, Aswathi Raveendran, Rokas Zalneravicius, Giedre Grinciene, Agne Mikalauskaite

Center for Physical Sciences and Technology, Laboratory of Nanostructures, Vilnius, Lithuania
** simonas.ramanavicius@ftmc.lt*

Magnetic nanoparticles have attracted significant interest owing to their size-dependent physicochemical and magnetic properties, which enable a broad spectrum of technological and biomedical applications [1]. Among them, ferrite nanoparticles with a spinel crystal structure are particularly versatile, as the distribution of metal cations between tetrahedral and octahedral sites strongly influences key characteristics, including magnetic anisotropy, saturation magnetization, coercivity, and electron-transfer behavior. Even subtle variations in cation arrangement can induce pronounced changes in performance, enabling precise tailoring of material properties [2]. In addition to their well-established roles in catalysis, environmental remediation, sensing, and energy systems, ferrite nanomaterials have demonstrated considerable potential as antimicrobial agents, targeted drug delivery, magnetic resonance imaging (MRI) contrast agents, hyperthermia-based cancer therapy, biosensing, and water disinfection. Their superior chemical stability, resistance to oxidation, and corrosion tolerance, compared with metallic magnetic nanoparticles, further enhance their suitability for applications in aqueous, oxidative, and biological environments [2,3].

In this study, ferrite nanoparticles were synthesized via a hydrothermal co-precipitation approach, and their properties were systematically tuned through surface chemical modification. Comprehensive characterization was carried out using transmission electron microscopy (TEM), X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and Raman spectroscopy. The relationship between synthesis parameters, surface functionalization, and the resulting structural, magnetic, and functional properties of the ferrite nanoparticles is discussed, emphasizing their adaptability for multifunctional and application-specific design.

Acknowledgements. This project received funding from the Research Council of Lithuania (LMTLT), agreement No S-MIP-24-14.

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FLEXIBLE PAPER ELECTRODES WITH ULTRAHIGH CAPACITANCE AND LONG-LIFE AT PRACTICAL MASS LOADING FOR BATTERY SUPERCAPACITOR HYBRID

Man Singh[1]*, Alankar Kafle[1], Divyani Gupta[1], Tharamani C. Nagaiah[1]

[1] Indian Institute of Technology Ropar, Punjab, India
* *man.singh@ftmc.lt*

Designing economic and bio-degradable flexible electrodes with industry-standard mass loading (>10 mg cm^{-2}) poses significant challenges for stable and durable energy storage devices. In this work, an endeavor is made to design flexible and bio-degradable laboratory filter paper-based electrodes for eco-friendly and economical flexible battery supercapacitor hybrids (BSHs) via a combination of electroless and electrodeposition techniques. Filter paper (FP) is made conductive by electroless deposition of NiB-layer (Ni/NiB-FP) on which high mass loadings of nickel iron phosphide active material (upto 17 mg cm^{-2}) are deposited via electrodeposition method to obtain NiFeP@Ni/NiB-FP flexible electrodes. The developed NiFeP@Ni/NiB-FP electrode (17 mg cm^{-2}) undergoes electrochemical activation by surface reconstruction to achieve ultrahigh areal capacitance of 37.5 F cm^{-2} (18.75 C cm^{-2}, 2220 F g^{-1})

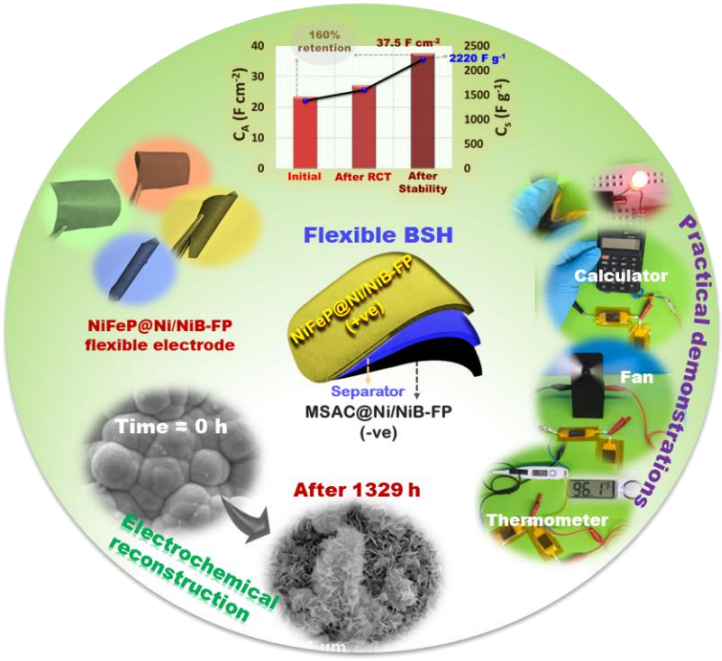

Fig. 1. Schematic representation of nickel iron phosphide deposited paper electrodes for flexible battery-supercapacitor hybrid

at 5 mA cm^{-2} as battery type electrode with exceptional rate capability (90.6% at 30 mA cm^{-2}) and ultrastable cycling retaining 37.4 F cm^{-2} at 5 mA cm^{-2} even after continuous cycling for 1329 h (≈55 days). As a proof of concept, a tandem device with four flexible paper-based BSH cells in series is demonstrated to achieve stable operational voltage up to 6 V. Practical applicability is showcased by powering a panel with 50 LEDs (each rated 1.6 V), a small fan, a digital calculator and a digital thermometer while measuring the body temperature highlighting the versatility for diverse applications.

Acknowledgement. M.S. and A.K. contributed equally to this work.

ASCORBIC ACID-ASSISTED MoS_x IMMOBILISED ALGINATE HYDROGELS FOR REALISTIC ORGANIC POLLUTANT REMOVAL

Gabriele Sarapajevaite [1]*, Aldona Balciunaite[1], Paola Fabbri[2,3], Davide Morselli[2,3], Jurga Juodkazyte[1]

[1] Center for Physical Sciences and Technology, Vilnius, Lithuania
[2] Civil, Chemical, Environmental and Materials Engineering Department, Bologna, Italy
[3]National Interuniversity Consortium of Materials Science and Technology (INSTM), Firenze, Italy
** gabriele.sarapajevaite@ftmc.lt*

The contamination of wastewater by synthetic dyes from industrial effluents remains a significant environmental concern, particularly at the low concentrations typical of real systems [1]. Molybdenum sulfide (MoS_x) is a promising adsorbent due to its layered structure, high surface area, and abundance of active sites, such as defects or unsaturated sulfur species, that enable efficient pollutant removal [2]. This study aimed to develop a more sustainable synthesis route for MoS_x using ascorbic acid as a green reducing agent and systematically investigate the effects of its concentration (0.3–0.5 M) and temperature (200–220 °C) on material properties and adsorption performance. Moreover, MoS_x was incorporated into an alginate-based hydrogel to produce an easily processable adsorbent, and the adsorption performance of the resulting composite hydrogels for methylene blue removal was evaluated.

The results demonstrate that ascorbic acid effectively enables MoS_x formation, with higher concentrations yielding materials with greater surface area and improved adsorption capacity. The maximum methylene blue adsorption capacity reached 48.3 mg g^{-1}, with 96.4% removal within 120 min. Immobilization in alginate hydrogels facilitated handling, separation, and reuse, while maintaining effective dye removal at low concentrations and showing improved performance upon reuse. Adsorption followed Langmuir and Temkin isotherm models. XPS analysis indicated that during adsorption methylene blue interacts primarily with COOH groups in the alginate matrix. Desorption studies revealed stronger dye retention in composite hydrogels compared to neat alginate. Overall, this work presents a sustainable and practical approach for efficient dye removal from realistic wastewater systems.

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THE ELIMINATION OF THE NEGATIVE IMPACT OF ZINC IN PORTLAND CEMENT BY ACCELERATING CONCRETE ADMIXTURES

Pavel Šiler*, Ondřej Kunovský, Vojtěch Florian, František Šoukal

Institute of Materials Science, Brno University of Technology, Brno, Czech Republic
* siler@fch.vut.cz

Thank to benefits from economic and ecological point of view the secondary raw materials like slag are also used. Due to increasing use of secondary products containing zinc, the amount of zinc in the clinker and secondary raw materials is increasing in recent years. Portland clinker can gain zinc from solid waste or tires which are widely used as fuel for a burning in rotary kiln. In the case of secondary raw materials, zinc may be present in the primary material, where the manufacturing process leads to its removal and concentrating to "waste" which is used in the cement industry. The biggest problem with cement dopped with zinc is the retardation of hydration and decreasing of mechanical properties which is already causing problems in cement plants. The main objective of this presentation is to show how the use of suitable types of hydration accelerators can help to eliminate negative effects of zinc on cement.

BALANCING NUTRIENTS RECOVERY AND HEAVY METALS RISK IN MUNICIPAL SOLID WASTE COMPOST: A PARTICLE–SIZE PERSPECTIVE

Bilal Touseef[1]*, Gintaras Denafas[1], Karolina Barcauskaite[2], Sana Ullah[2]

[1]Department of Environmental Technology, Kaunas University of Technology, Kaunas, Lithuania
[2]Research Centre for Agriculture and Forestry, Lithuania,
* *bilal.touseef@ktu.edu*

Municipal solid waste (MSW) compost is becoming a widely accepted sustainable solution to manage urban waste. It has the potential to be used in agriculture as a soil enhancer and quasi–fertilizer. However, its agronomic use is frequently limited by the presence of heavy metals, which are caused by the mixed waste streams. Although extensive studies have been conducted on the quality of MSW compost, very little effort has been made to evaluate the influence of particle–size fractionation on the regulation of nutrients and heavy metals distribution. Bulk compost properties are studied in most existing research, thereby ignoring intra–sample heterogeneity, which may be a critical factor for agronomic value and contamination risk. As a result, the potential of size–based separation as a method to maximize the quality and safety of compost has not been adequately investigated.

This paper compares the composition of nutrients and heavy metals in different granulometric fractions of MSW compost generated by mechanical–biological treatment facilities in Kaunas, Alytus (Lithuania), and Daugavpils (Latvia). The compost samples were separated into six particle size classes (>5, 5–2.5, 2.5–1, 1–0.5, 0.5–0.2, and <0.2 mm) and physiochemically characterized. Inductively coupled plasma–optical emission spectroscopy (ICP–OES) was used to measure nutrients (Ca, K, Mg, and P) and heavy metals (Cd, Cr, Cu, Ni, Pb, and Zn) in triplicate.

Our findings indicate that the distribution is evidently dependent on the size of compost particles. The increase in nutrient and heavy metal content was found in fine fractions (< 1 mm), but coarse fractions contained mainly inert physical impurities, in particular, glass. There were also regional differences: the compost in Kaunas met the necessary quality standards according to EU regulations in all fractions, but in Alytus and Daugavpils only the coarse ones (>2.5 mm) could be used in agriculture, dependent upon the removal of physical contaminants. Alytus fine fractions had more of the heavy metals in question and Daugavpils samples were over in Cd, Cu, Ni, and Zn. Although the finer fractions were richer in nutrients, the excessive amount of heavy metals present makes their safe application in agriculture restricted.

These outcomes imply a key trade–off between the recovery of nutrients and the threat of contamination. The separation of particles, especially removing fine fractions (< 1 mm) and inert impurities in coarse fractions can significantly enhance the quality of compost. Overall, the particle–size–based management is a feasible strategy to enhance the safety and reuse capability of MSW compost in agriculture.

S-ALKYLATED OXADIAZOLE SYNTHESIS AND EVALUATION OF PROPERTIES

Ieva Bartkevičiūtė[1]*, Vida Malinauskienė[1], Asta Žukauskaitė[2], Alena Kadlecová[2], Tomáš Jirsa[2], Vilija Kederienė[1]

[1] Faculty of Chemical Technology, Kaunas University of Technology, Kaunas, Lithuania
[2] Faculty of Science, Palacký University Olomouc, Olomouc, Czech Republic
* *ieva.bartkeviciute@ktu.lt*

The spectrum and application areas of compounds exhibiting biological activity are wide, but considering the resistance of pathogens, the potential toxicity of agents, the lack of efficiency or precision of action, there remains a great need for obtaining new biologically active compounds [1]. Oxadiazole and its various derivatives are characterized by exceptionally favourable chemical, physical, pharmacokinetic properties, excellent opportunities to form interactions with macromolecules, sufficient compatibility of reactivity and stability. A growing interest is devoted to analogues of 1,3,4-oxadiazoles with substituents in the second and fifth positions, and it is becoming an important topic of medicinal chemistry research [2,3]. After examining the potential of this class of compounds, it was decided to expand the compound library in the hope of obtaining compounds with biological activity.

The research was started with the preparation of oxadiazole thiol, a precursor of the target compounds, according to known principles [4]. The further synthesized oxadiazole thiol was treated with benzyl halides under basic reaction conditions and the target alkylated oxadiazole derivatives were obtained in good yields. Detailed spectroscopic studies confirmed the structures and high purity of the target compounds.

Parasitic nematodes and worms that infect plants, animals or humans have a negative impact on the quality of life and may cause significant economic losses. Helminths are becoming more resistant to known drugs and treatment methods, making it difficult to effectively control parasitic infections in agriculture, medicine, and veterinary medicine, making it very important to develop new compounds with anthelmintic effects [5]. Literature analysis suggests that oxadiazole derivatives may also exhibit anthelmintic properties [6]. It was decided to evaluate the properties of the synthesized compounds using model nematodes *C. elegans*. Using the chitinase test, it was determined that two synthesized compounds had a greater influence on the development of the model nematode, while the others showed varying degree of activity.

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CARBAZOLE-BASED PHOSPHONIC ACID DERIVATIVES: STRUCTURE–PROPERTY CORRELATIONS

Aida Drevilkauskaitė[1*], Lea Zimmermann[2], Eike Köhnen[2], Vytautas Getautis[1], Steve Albrecht[2], Artiom Magomedov[1]

[1] Department of Organic Chemistry, Kaunas University of Technology, Kaunas, Lithuania
[2] Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Young Investigator Group Perovskite Tandem Solar Cells
* *aida.drevilkauskaite@ktu.edu*

Small phosphonic-acid molecules used as self-assembled monolayers (SAMs) are widely applied in p-i-n perovskite solar cells (PSCs) [1]. However, the relationship between molecular structure and device performance is still not fully understood, even though many different molecular designs exist. Previous studies have shown that changes in the chromophore, linker, anchoring group, or side groups can affect device performance [2,3]. Still, direct comparisons are difficult because different studies use different perovskite compositions, device structures, and small sets of molecules.

Here, we study nine carbazole-based phosphonic acid derivatives using the same perovskite solar cell architecture [4]. We investigate how different substitution patterns on the carbazole core influence device properties. Molecules with phenyl, methyl, and methoxy groups at different positions were synthesized and used as SAM interlayers.

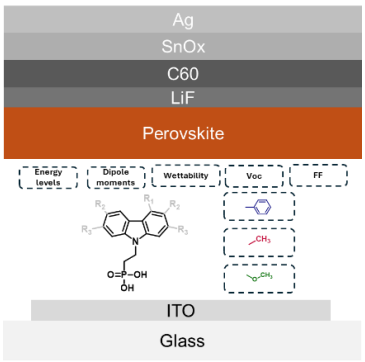

Fig. 1. Schematic illustration of the p-i-n PSC architecture incorporating carbazole-based SAMs with different functional groups

We find that derivatives substituted at the 3,6-positions show higher fill factors and better power conversion efficiencies compared to other positions. We also observe a relationship between ionization potential and fill factor, suggesting an optimal energy level range for best performance. Overall, the results show that small changes in molecular structure can strongly affect device performance and provide useful design rules for future SAM materials in perovskite solar cells.

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FUNCTIONAL ROOM-TEMPERATURE PHOSPHORESCENT MATERIALS FOR OXYGEN SENSING AND EMISSIVE TAG APPLICATIONS

Lukas Dvylys*, Rasa Keruckienė, Juozas Vidas Gražulevičius

Department of Polymer Chemistry and Technology, Kaunas University of Technology, Lithuania
** lukas.dvylys@ktu.edu*

Room-temperature phosphorescence (RTP) demonstrated by organic materials has attracted significant attention due to its long-lived emission from triplet excited states and its sensitivity to molecular oxygen [1]. Unlike fluorescence, RTP is efficiently quenched by oxygen, making it highly suitable for applications requiring controlled emission, such as sensing and optical information technologies [2].

Recent advances in the development of purely organic RTP systems have enabled materials with tuneable emission, improved processability, and lower toxicity compared to the corresponding characteristics of metal-complexes-based counterparts [3]. Efficient RTP is typically achieved by promoting intersystem crossing and stabilizing triplet states through molecular design strategies, including the incorporation of heteroatoms, rigid frameworks, and donor–acceptor architectures [1,4].

In this work, two structurally distinct families of organic RTP materials are presented. Thianthrene-based derivatives were developed as oxygen-responsive systems, where sulphur atoms enhance spin–orbit coupling and facilitate efficient triplet formation, enabling phosphorescence to respond sensitively to changes in oxygen concentration [5]. In parallel, donor–acceptor compounds incorporating phenoxathiin and quinoxaline units were synthesized to achieve tuneable, persistent emission for emissive tagging applications. The phenoxathiin moiety promotes intersystem crossing and triplet stabilization, while the molecular design allows control over photophysical properties [6].

The synthesized compounds were investigated in terms of their thermal, electrochemical, and photophysical properties, demonstrating how targeted molecular design enables functional RTP materials for oxygen sensing and emissive tagging applications.

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DONOR-CONTROLLED TRIPLET PATHWAYS IN DIBENZO[*A,C*]IMIDAZOPHENAZINE EMITTERS FOR HIGH-EFFICIENCY OLEDS

Aliyu Mohammed Hamisu[1]*, Viktorija Andruleviciene[1], Matas Guzauskas[1], Muhammad Faisal Khyasudeen[2], Kai Lin Woon[2], Dmytro Volyniuk[1], Azhar Ariffin[3], Juozas Vidas Grazulevicius[1]

[1]Department of Polymer Chemistry and Technology, Kaunas University of Technology, Kaunas, Lithuania
[2]Low Dimensional Material Research Centre, Department of Physics, University Malaya, Kuala Lumpur, Malaysia
[3]Department of Chemistry, University Malaya, Kuala Lumpur, Malaysia
** hammoh@ktu.lt*

Efficient triplet harvesting is crucial for achieving high-performance purely organic OLEDs, yet it requires precise control over excited-state topology, radiative efficiency, and charge transport. Here, donor selection on a rigid dibenzo[a,c]imidazophenazine (DBIPO) core enables precise control of triplet-harvesting pathways in purely organic emitters. Three derivatives illustrate distinct mechanisms: EHBIPOAz shows HLCT behavior with minimal reorganization ($\lambda \approx 0.084$ eV) and ultrafast hot-exciton RISC ($k_{hRISC} \geq 10^{11}$ s^{-1}), EHBIPOAc exhibits efficient TADF from a stabilized CT state, and EHBIPOPh combines TADF with vibronically assisted upconversion. All materials feature high PLQY (75-97%), robust thermal stability ($T_{d,5\%}$ > 440 °C), and balanced bipolar transport. In OLEDs (5 wt% in 5tCzBN), they achieve EQEs of 23.4%, 25.5%, and 28.7%, respectively. These results establish donor-driven design as an effective strategy to access HLCT, TADF, or hot-exciton pathways while maintaining high device efficiency.

ISOPHTALOYLBISDIBENZOTHIOPHENE: A NOVEL SCAFFOLD FOR THE DEVELOPMENT OF EFFICIENT TRIPLET EMITTERS

Alena Kimpel*, Mariia Stanitska, Oleksandr Bezvikonnyi, Dmytro Volyniuk, Juozas Vidas Grazulevicius

Department of Polymer Chemistry and Technology, Kaunas University of Technology, Kaunas, Lithuania
* *alena.kimpel@ktu.edu*

The presented work is on the study of the effects of crystallinity and management of triplet excitations of the derivatives of isophtaloylbisdibenzothiophene as a central electron-withdrawing core and various peripheral donor moieties such as diphenylamine, dimethylacridine, carbazole, and phenoxazine. The compounds exhibit high thermal stability, with the 5% weight loss temperatures varying from 445 to 525 °C. The derivative with phenoxazine donor units is a crystalline organic semiconductor (COS) as determined by differential scanning calorimetry and analysis of the morphology of the films. Ionization energies of the compounds range from 5.4 to 5.9 eV, depending on the donor strength. The analysis of PL spectra and decay curves of the films of the compounds doped in Zeonex recorded at the different temperatures point to the probable interplay of room temperature phosphorescence and thermally activated delayed fluorescence. The phosphorescence of the COS is blue-shifted when compared to the fluorescence. Its lifetime is in the range of seconds for both liquid and solid samples. The white organic light emitting diode fabricated utilizing the sky-blue Iridium complex FIrpic and the COS as a host for the red fluorescent emitter exhibits the color rendering index of up to 80 and the CIEx,y coordinates of (0.31, 0.34)-(0.33, 0.36) at the different voltages. The corresponding color correlated temperature ranges from 6115 to 7110 K. The obtained values are close to the CIE standard illuminant D65 of the white light.

PYRIDO[2,3-*B*]PYRAZINE DERIVATIVES AS DONOR-ACCEPTOR TYPE EMITTERS EXHIBITTING THERMALLY ACTIVATED DELAYED FLUORESCENCE FOR HIGH-EFFICIENCY OLEDS

Domantas Lekavičius*, Rasa Keruckienė, Matas Gužauskas, Dmytro Volyniuk, Juozas V. Gražulevičius

Kaunas University of Technology, Kaunas, Lithuania
** domantas.lekavicius@ktu.lt*

Organic emitters exhibiting thermally activated delayed fluorescence (TADF) have become very important alternatives to phosphorescent metal complexes used in organic light-emitting diodes (OLEDs). The recent work has shown that OLEDs based on purely organic TADF materials can be used in many fields, such as advanced displays and lighting devices. TADF emitters are of relatively low-cost and environmentally friendly [1]. However, development of TADF emitters with high efficiency and specific colors of emission, especially for high-performance OLEDs, is still an area of active research.

In this investigation, the photophysical properties and possible uses of new derivatives of pyrido[2,3-b]pyrazine linked through a phenyl linker to either carbazole or phenothiazine fragments that showed efficient TADF are reported. Their ability to absorb and emit light, photoluminescence quantum yields, the lifetimes of their excited states, and the energy difference between their excited singlet and triplet states (ΔE_{ST}) are discussed. The studied materials show TADF, facilitated by efficient reverse intersystem crossing due to small ΔE_{ST} values (as low as 0.16 eV). The emission spans from green to orange with quantum yields of the solid solutions in Zeonex of up to 82%.

The application of the newly synthesized TADF emitters in OLEDs was explored. The devices fabricated with the emissive layer of non-doped emitters showed external quantum efficiency (EQE) of 0.94%. Through optimization by using a host-guest system, the EQE was significantly improved. It reached up to 21.3 %, accompanied by a high current efficiency of 52.5 cd/A and a brightness of 7202 cd/m². The achieved device efficiencies are close to the theoretical limit for TADF OLEDs [2].

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DESIGN AND SYNTHESIS OF NOVEL PYRAZOLE-ISOXAZOLE DERIVATIVES

Ineta Meldaikytė*, Eglė Arbačiauskienė, Algirdas Šačkus, Vilija Kederienė

Department of Organic Chemistry, Kaunas University of Technology, Kaunas, Lithuania
* *ineta.meldaikyte@ktu.edu*

Pyrazole and isoxazole derivatives are biologically active compounds of importance in medicinal chemistry. Several drugs are known to contain scaffolds of pyrazole or isoxazole: *Cloxacillin*, *Celecoxib*, *Ibotenic*, and *Lonazolac* [1]. Various pyrazole-isoxazole compounds exhibit synergistic antifungal activity in combination with *Voriconazole* against *C. albicans* [2]. There is not much information in the literature on isoxazole[5,4-*d*]pyrimidin-4-amine, but some of these compounds have been found exhibit inhibitory effects on the vascular endothelial growth factor receptor and platelet derived growth factor receptor [3].

In this work, we synthesized a series of pyrazole-isoxazole derivatives (Fig. 1.). Some of these compounds were obtained by attaching different acetylene or allyl groups containing reagents.

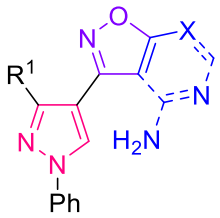

Fig. 1. General structure of new pyrazole-isoxazole derivatives

The resulting derivatives were then functionalized using Pd-catalyzed Suzuki-Miyaura reaction conditions. A new series of pyrazole-isoxazole[5,4-*d*]pyrimidin-4-amine compounds was also obtained using an inexpensive and simple methodology.

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CARBORANE DERIVATIVES AS ELECTRON-TRANSPORTING MATERIALS FOR PEROVSKITE SOLAR CELLS

Julius Petrulevicius[1]*, Lea Zimmermann[2], Wander Max Bernardes de Araujo[2], Maxim Simmonds[2], Arman Mahboubi Soufiani[2], Maryte Daskeviciene[1], Tadas Malinauskas[1], Giedre Bubniene[1], Giedrius Juska[3], Vygintas Jankauskas[3], Dorothee Menzel[2], Florian Scheler[2], Eike Köhnen[2], Lars Korte[2], Bernd Stannowski[2], Jona Kurpiers[2], Steve Albrecht[2], Vytautas Getautis[1]

[1] Department of Organic Chemistry, Kaunas University of Technology, Kaunas, Lithuania
[2] Solar Energy Division, Helmholtz-Zentrum Berlin, Berlin, Germany
[3] Institute of Chemical Physics, Vilnius University, Vilnius, Lithuania
** julius.petrulevicius@ktu.lt*

The development of perovskite solar cells (PSCs) has accelerated significantly with efficiencies reaching 27.3%, which is comparable to silicon. The efficiencies of perovskite/silicon tandem solar cells have reached 35.0%, which is even higher than the theoretical limits of single-junction silicon solar cells [1]. Buckminsterfullerene (C_{60}) is widely used as an electron-transporting material (ETM) in high-efficiency PSCs because it efficiently extracts electrons and has high electron mobility. Nevertheless, C_{60} also has some disadvantages, which include high cost, interfacial non-radiative recombination, high parasitic absorption, and lack of mechanical stability leading to separation of layers. Organic ETMs have recently attracted much attention as an alternative to fullerene C_{60} due to their low cost, facile synthesis as well as better adhesion with perovskite.

In this work, a novel carborane-based ETMs were designed and synthesized (Fig. 1) via a simple three-step synthesis procedure.

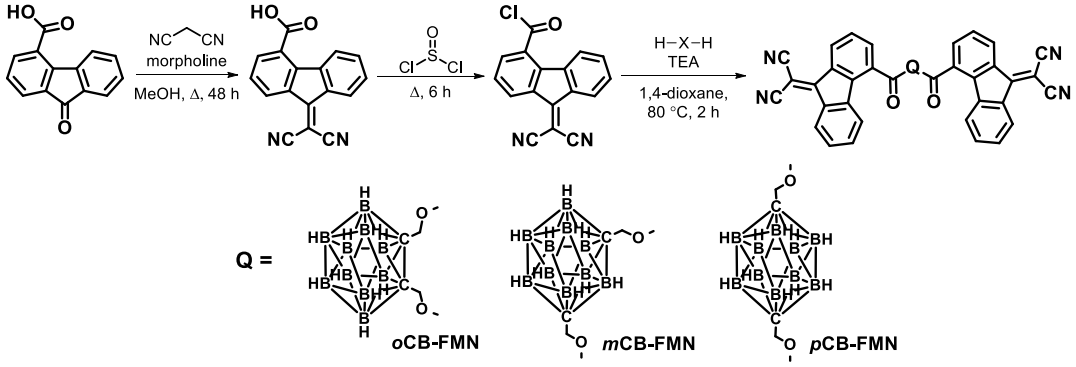

Fig. 1. Synthesis of carborane-based ETMs

The electron mobility of *o*CB-FMN, *m*CB-FMN and *p*CB-FMN was found to be 1×10^{-5}, 5×10^{-5}, and 5×10^{-6} cm^2/Vs at zero-electric field. The new materials were tested as ETMs and successfully applied in single-junction PSCs and perovskite/silicon tandem solar cells.

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SINGLE COMPONENT WHITE LIGHT EMISSION USING SMALL ORGANIC COMPOUNDS

Ehsan Ullah Rashid[1*], Rishika Suresh[2], Dmytro Volyniuk[1], Sathiyanarayanan Kulathu Iyer[2], Juozas Vidas Grazulevicius[1]

[1]Department of Polymer Chemistry and Technology, Kaunas University of Technology, Kaunas, Lithuania
[2]School of Advanced Sciences, Vellore Institute of Technology University, Vellore, India
*ehsan.rashid@ktu.lt

Single-component white emitters are useful for simplifying white organic light-emitting diodes (OLED) structures and avoiding the charge-balance and interfacial losses that often limit conventional multilayer RGB devices [1]. In this work, we report a rationally designed organic emitter that shows white emission through a dual emissive state mechanism. Photophysical analysis shows that the blue emissive component originates from the intramolecular charge-transfer (CT) excited state of the monomer, whereas the yellow component arises from excimer formations. The interplay between these two emissive channels enables balanced white-light generation. To analyze the nature of emissive excited-state, quantum chemical calculations were performed. The calculated first singlet excited-state energy levels and wavefunction distributions of the monomer and dimer (Fig. 1) reveal clear differences in excited-state localization, supporting the coexistence of high energy monomeric CT state and low-energy excimer state.

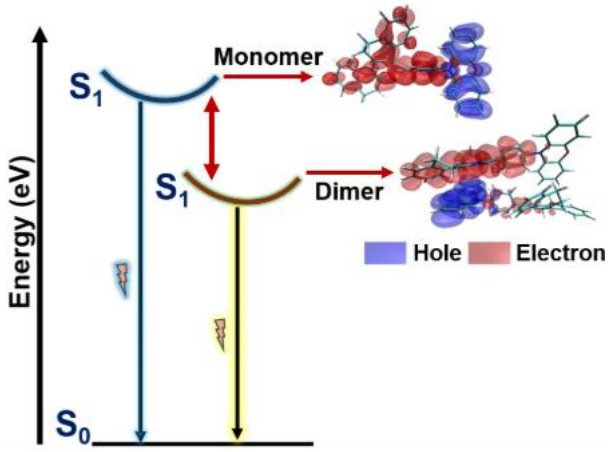

Fig. 1. Computed first singlet (S_1) excited state energy levels and wave functions of monomer and of dimer of organic emitter

A non-doped OLED fabricated with this emitter as the emissive layer showed broadband electroluminescence close to white light, whereas a doped OLED, in which intermolecular interactions were suppressed, showed blue emission. These results establish molecular aggregation control as an effective route to color-tunable and structurally simplified OLEDs.

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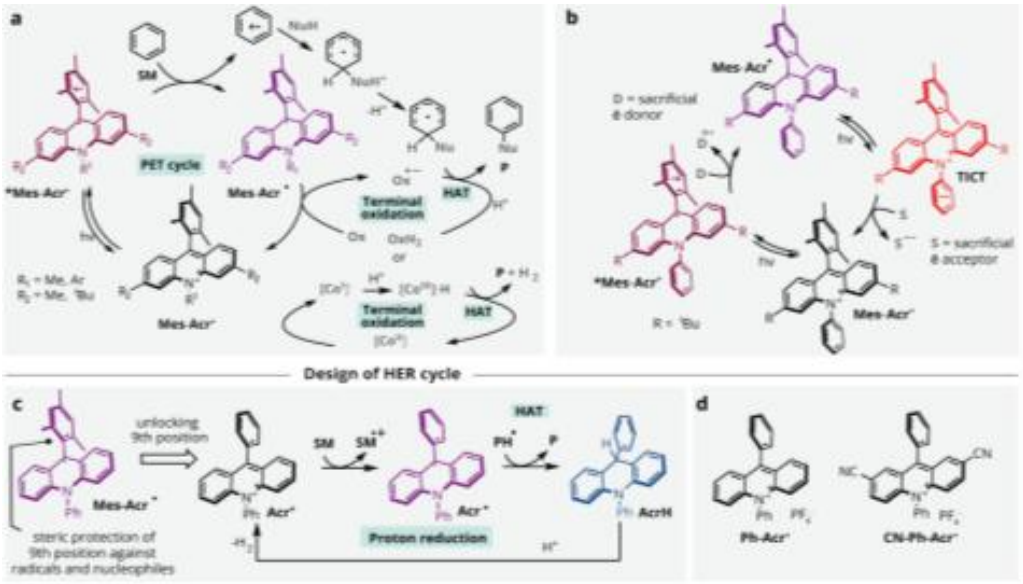
PHOTOREDOX MANIFOLD FOR DEHYDROGENATIVE COUPLING USING PROTONS AS OXIDANTS

Jonas Žurauskas[1]*, Paulius Vaickūnas[1], Gustautas Snarskis[3], Nojus Radzevičius[1], Barbara Chatinovska[1], Gediminas Kreiza[2], Steponas Raišys[2], Mantas Šimėnas[2], Vidmantas Kalendra[2], Kęstutis Zakarauskas[4], Karolis Kazlauskas[2], Edvinas Orentas[1]

[1] Vilnius University, Department of Organic Chemistry, Vilnius, Lithuania
[2] Vilnius University, Faculty of Physics, Vilnius, Lithuania
[3]Biomatter, Business Stadium West, Vilnius, Lithuania
[4]Lithuanian Energy Institute, Kaunas, Lithuania
** jonas.zurauskas@chgf.vu.lt*

The direct coupling of two unfunctionalized molecules under mild conditions embodies an ideal in synthetic chemistry [1-3]. In this study, we report a metal-free photocatalytic process for arene C-H functionalization that employs an acridinium-type catalyst and produce dihydrogen as the only by-product. Throughout the catalytic cycle, the catalyst acts as an oxidizing agent, a hydrogen atom transfer agent, and a proton-reducing agent, enabling a cross-dehydrogenative transformation without the need for external oxidants. The reaction is conveniently performed using visible light, and the high oxidation potential of the catalyst allows it to engage even electron deficient arene substrates. The catalytic mechanism disclosed in Figure 1 can become a general logic for developing various cross-dehydrogenative reactions adaptable for pharmaceutical and material sciences.



Mes – mesityl;
SM – starting material;
P-– product.

Fig. 1. Established and hypothesized reactivity modes of acridinium photocatalysis: a – a photocatalytic cycle based on reductive photocatalyst quenching, when the regeneration of the catalyst is achieved either by sacrificial oxidant or cobalt-mediated dihydrogen formation; b – exploration of excited acridine radical as a potent reductant; c – design of acridinium catalyst for hydrogen atom transfer and proton reduction to produce dihydrogen during the turnover (HER cycle); d – chemical structures of the photocatalysts.

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NOVEL 3-ETHYLCARBAZOLE-BASED HOSTS FOR HIGH EFFICIENCY OLEDS

Saulius Grigalevicius[1]*, Dovydas Blazevicius[1], Mantas Kirstukas[1], Raminta Beresneviciute[1], Chih-Hung Ko[2], Cai-Fan Lo[2], Chih-Hao Chang[2]

[1] Department of Polymer Chemistry and Technology, Kaunas University of Technology, Kaunas, Lithuania
[2] Department of Electrical Engineering, Yuan Ze University, Taoyuan, Taiwan
* *saulius.grigalevicius@ktu.lt*

In recent years, organic light-emitting diodes (OLEDs) have attracted strong interest from both academia and industry because of their design versatility and potential as efficient, sustainable light sources, creating an ever-growing demand for new high-performance materials. Carbazole represents one of the most used electron-donating fragments in host design due to its high triplet energy, thermal stability, favorable charge-transport properties, and extensive functionalization potential. To further achieve these properties, carbazole units are typically combined with suitable electron acceptors, which play a decisive role in defining the photophysical and charge-transport characteristics of the host materials [1-3].

In this study, four new ethylcarbazole-based host materials, CzeCzS, eCz2S, CzeCzM, and eCz2M, were successfully synthesized by combining carbazole electron donors with either diphenylmethanone or dihenyl sulfone electron acceptors and were evaluated for their suitability in OLED applications. The structures of compounds are shown in Figure 1.

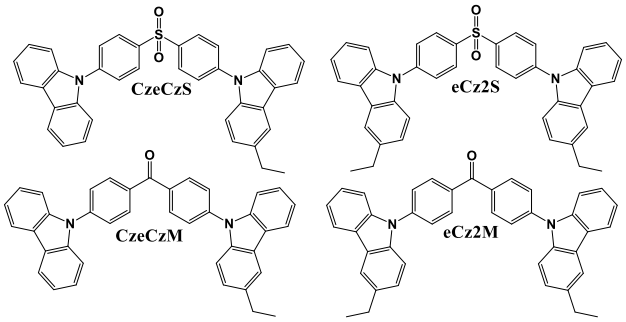

Fig. 1. Structures of compounds CzeCzS, eCz2S, CzeCzM, and eCz2M

The experimental results revealed that these compounds can effectively serve as hosts for both green phosphorescent and yellow thermally activated delayed fluorescence (TADF) OLEDs. The best performing device, based on the eCz2M: B3PyMPM co-host system, achieved an external quantum efficiency (EQE) of 20.3%, a luminance efficiency (CE) of 72.7 cd/A, and a power efficiency (PE) of 95.1 lm/W. Also, for the yellow-emitting TADF OLED prototype, our co-host systems enabled to achieve an EQE of 10.3%.

Acknowledgements. This work was supported by the Research Council of Lithuania (Grant No. S-MIP-25-23) and Kaunas University of Technology. C.H.C. gratefully acknowledges the funding support from the National Science and Technology Council of Taiwan, under the grant numbers (NSTC 112-2923-E-155-002-MY4, NSTC 113-2221-E-155-014-MY3, and NSTC 114-2923-E-155-001-MY3).

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IN SILICO PREDICTION OF ADMET PARAMETERS FOR 2*H*,5*H*-CHROMENO[4',3':4,5]THIOPYRANO[2,3-*d*]THIAZOL-2-ONE DERIVATIVES

Maryna Stasevych[1]*, Mykhailo Hoidyk[1,3], Viktor Zvarych[2], Andriy Karkhut[1], Svyatoslav Polovkovych[1], Roman Lesyk[3]

[1] Department of Technology of Biologically Active Substances, Pharmacy and Biotechnology, Lviv Polytechnic National University, Lviv, Ukraine,
[2] Department of Automated Control Systems, Lviv Polytechnic National University, Lviv, Ukraine,
[3]Department of Pharmaceutical, Organic and Bioorganic Chemistry, Danylo Halytsky Lviv National Medical University, Lviv, Ukraine
** maryna.v.stasevych@lpnu.ua*

In modern medicinal chemistry, the development of novel antiepileptic drugs (AEDs) increasingly relies on the early identification of pharmacokinetic liabilities to reduce attrition rates in later clinical stages. Consequently, comprehensive ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) profiling has become an indispensable tool for rational drug design. This study aimed to conduct an *in silico* ADMET profiling of a library of 448 novel 2*H*,5*H*-chromeno[4',3':4,5]thiopyrano[2,3-d]thiazol-2-one derivatives (Figure 1) to identify hit structures with an optimal balance of safety and efficacy for the synthesis. The investigation utilized the *ADMET-AI* platform [1].

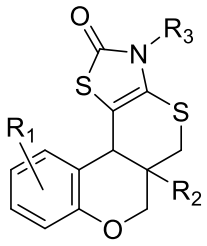

Fig. 1. General structure of library

The methodology included calculating drug-likeness descriptors for primary screening, followed by a comparative statistical analysis of the top selected structures against approved AEDs and reference compounds. The screening identified 20 promising candidates demonstrating high intestinal absorption and blood-brain barrier permeability, which is critical for CNS-active agents. Toxicological profiling revealed that these structures possess significantly lower mutagenic and carcinogenic potential compared to the reference thiazolidinones. However, specific pharmacokinetic challenges were identified.

In conclusion, the *in silico* results confirm the high potential of the thiopyrano[2,3-d]thiazole scaffold for developing safer anticonvulsants. Nevertheless, further lead optimization is required to decrease lipophilicity, improve metabolic stability, and mitigate potential hepatotoxicity risks prior to advancing to *in vivo* trials.

Acknowledgements. The study was carried out within the framework of the research project "Search for novel potential anticonvulsant agents for the treatment of post-traumatic epilepsy in military personnel and the civilian population", funded by the Ministry of Education and Science of Ukraine (Project registration number: 0125U001794).

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DESIGN AND BIOLOGICAL ASSESSMENT OF PYRIDINE-PYRROLIDINE-HYDRAZONE HYBRIDS SUPPORTED BY *IN SILICO* ADMET PREDICTION

Simona Talačkaitė[1], Ilona Jonuškienė[1], Kristina Kantminienė[2], Maryna Stasevych[3], Ingrida Tumosienė[1]*

[1] Department of Organic Chemistry, Kaunas University of Technology, Kaunas, Lithuania
[2] Department of Physical and Inorganic Chemistry, Kaunas University of Technology, Kaunas, Lithuania
[2] Department of Technology of Biologically Active Substances, Pharmacy, and Biotechnology, Lviv Polytechnic National University, Lviv, Ukraine
** ingrida.tumosiene@ktu.lt*

Heterocyclic compounds constitute a significant part of organic compounds in design and development of modern drugs due to their structural versatility and ability to modulate key biological targets. Among these, pyridine and pyrrole derivatives have attracted significant attention for their favourable physicochemical properties and broad therapeutic potential. Pyridine ring often enhances metabolic stability and binding specificity owing to its basicity, hydrophilicity, chemical stability, and the ability to form hydrogen bonds [1], while pyrrole scaffolds contribute unique electronic features that support diverse pharmacological activities [2].

In the present study, a series of hydrazones were synthesized from 1-(5-chloropyridin-2-yl)-5-oxopyrrolidine-3-carbohydrazide and variously substituted aromatic aldehydes [3]. Biological activity of the obtained novel hybrid 5-chloropyridine-5-oxopyrrolidine-hydrazone derivatives were evaluated by antioxidant and antibacterial assays. Among the tested molecules, hydrazone bearing *p*-dimethylbenzene moeity exhibited the strongest reducing properties and showed the highest antioxidant activity in both the FRAP and DPPH assays. In antibacterial tests, the same compound demonstrated the greatest inhibitory activity against *Escherichia coli* and *Bacillus subtilis* bacterial strains.

The ADMET properties of the synthesized compounds were evaluated *in silico* to predict their pharmacokinetic behavior and potential toxicity profiles. The prediction of ADMET (absorption, distribution, metabolism, excretion, and toxicity) parameters is a critical component of drug discovery and development, serving an essential role in the optimization of the pharmacokinetic properties of novel therapeutic compounds. The *in silico* analysis has indicated that the most active compound exhibits favorable logP and AMES properties, but it may have a potential risk of carcinogenicity.

Acknowledgements. This research has received funding from the Research Council of Lithuania (LMTLT), agreement No S-MIP-25-22.

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STRUCTURE AND PROPERTIES OF A ZINC(II) CHELATE COMPLEX WITH 2,6-DIPHENYL-4-(TRIFLUOROMETHYL)-1,3,5-OXADIAZINE

Savriyeva Nigina*

Bukhara State University, Bukhara, Republic of Uzbekistan
* *nigina.savriyeva@bk.ru*

Zinc(II) complexes with nitrogen- and oxygen-containing heterocyclic ligands attract considerable interest because of their structural diversity, biological relevance, and possible applications in medicine and materials science [1]. The introduction of fluorine-containing substituents, especially trifluoromethyl groups, can significantly affect the electronic properties, lipophilicity, and stability of the resulting coordination compounds [2]. Oxadiazine-type ligands formed through the cyclization of benzohydrazide derivatives are promising polydentate chelating agents for transition metal ions. The aim of this work was to synthesize and study a new zinc(II) chelate complex containing a 2,6-diphenyl-4-(trifluoromethyl)-1,3,5-oxadiazine fragment.

All reagents were of analytical grade and were used without further purification. The reaction mixture was stirred for 1 h. The precipitate formed was filtered off, washed with distilled water and cold ethanol, and dried under vacuum to give the target product. The interaction of zinc(II) acetate with N'-(3-hydroxy-3-phenyl-1-trifluoromethylpropyl)benzohydrazide in ammoniacal ethanol medium afforded a new zinc(II) chelate complex. Under the reaction conditions, cyclization of the hydrazone fragment is assumed to occur, resulting in a 2,6-diphenyl-4-(trifluoromethyl)-1,3,5-oxadiazine chelate system coordinated to the zinc center. The isolated product was obtained as a stable solid, indicating sufficient stability of the formed coordination compound. The molecular formula of the complex was established as $C_{17}H_{17}F_3N_3O_2Zn$ with a molecular weight of 417.72 g/mol. The elemental analysis data are presented in Table 1.

Table 1. Elemental analysis data for the zinc(II) complex $C_{17}H_{17}F_3N_3O_2Zn$ (M = 417.72 g/mol)

Element	**C**	**H**	**N**	**F**	**O**	**Zn**
Calculated (%)	48.88	4.10	10.06	13.64	7.66	15.65
Found (%)	48.88	4.10	10.06	13.64	7.66	15.65

The fluorine content confirms the presence of a trifluoromethyl substituent in the ligand framework, whereas the zinc content is consistent with the formation of a mononuclear zinc(II) complex. On the basis of the synthesis conditions and analytical data, the formation of a chelate structure involving an oxadiazine-type ligand can be proposed.

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STRUCTURAL AND THERMAL CHARACTERIZATION OF BIO-BASED VITRIMER

Viltė Šereikaitė*, Sigita Grauželienė, Jolita Ostrauskaitė

Department of Polymer Chemistry and Technology, Kaunas University of Technology, Kaunas, Lithuania
** vilte.sereikaite@ktu.lt*

Vitrimers were developed to overcome the main limitations of conventional polymers, particularly the permanent cross-linking of thermosets that prevents remelting and reprocessing, as well as the limited long-term stability of thermoplastics [1]. They belong to dynamic covalent networks (CANs), in which reversible bond exchange can be activated by external stimuli such as heat, pH, or UV light, enabling rearrangement of the polymer network. Among CANs, vitrimers are especially attractive because they can reorganize their network topology through exchange reactions—most commonly transesterification—without depolymerization (Fig. 1) [2]. Above the topology freezing transition temperature, reversible bond exchange reactions become active, allowing vitrimers to exhibit properties such as self-healing, recycling, repairability, and shape memory [3].

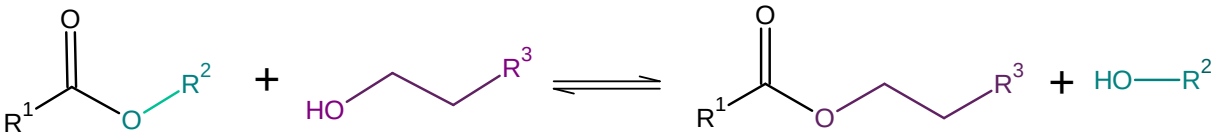

Fig. 1. Principle of transesterification reaction

In this study, vitrimers were synthesized via radical photopolymerization of resins containing plant-based monomers and comonomers. Ethyl-(2,4,6-trimethylbenzoyl)-phenylphosphinate was used as the photoinitiator. The chemical structure and vitrimer network formation were confirmed by Fourier transform infrared (FTIR) spectroscopy, which showed characteristic absorption bands and confirmed cross-linking. The cross-linking density of the vitrimer networks was evaluated using Soxhlet extraction and swelling tests, providing information on the degree of network formation and structural integrity. Thermal properties were investigated by thermogravimetric analysis (TGA) and dynamic mechanical thermal analysis (DMTA) to determine the thermal decomposition temperature (T_d), glass transition temperature (T_g), and topology freezing temperature (T_v). The determination of T_v is particularly important for vitrimer materials, as it defines the temperature at which the polymer network transitions from a viscoelastic solid to a viscoelastic liquid due to reversible bond exchange reactions. These results confirm the formation of thermally stable, dynamic networks, demonstrating the potential of bio-based photocurable materials for repairable and reprocessable applications.

Acknowledgements. This research was funded by the Research Council of Lithuania (project No. S-MIP-25-3).

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INFLUENCE OF BINARY SUPPLEMENTARY CEMENTITIOUS MATERIAL FROM EPSOM SALT PRODUCTION WASTE AND METAKAOLIN ON THE COMPRESSIVE STRENGTH OF PORTLAND CEMENT

Irmantas Barauskas*, Rimvydas Kaminskas, Emilis Saldžiūnas

Kaunas University of Technology, Kaunas, Lithuania,
** irmantas.barauskas@ktu.lt*

This study explored the potential of using the waste from Epsom salt production (ESW) and the metakaolin (MET) mix as a binary supplementary cementitious material (SCM) [1, 2]. Main chemical composition of ESW (wt.%): SiO_2 - 88.35, Al_2O_3 - 0.10, Fe_2O_3 - 2.47, MgO - 2.64. ESW and MET were mixed in different proportions and 25 wt.% of ordinary Portland cement (OPC) was replaced with these mixtures. The composition of the samples is presented in Table 1. The compressive strengths test of the specimens (Fig. 1), along with XRD analysis, were evaluated. The mixture investigated, regardless of the mixing proportions, was estimated to accelerate the early hydration of Portland cement and promote a strong pozzolanic reaction.

Table 1. Composition of samples

Sample no.	wt.%		
	OPC	ESW	MET
1	100	0	0
2	75	0	25
3	75	6.25	18.75
4	75	12.5	12.5
5	75	18.75	6.25
6	75	25	0

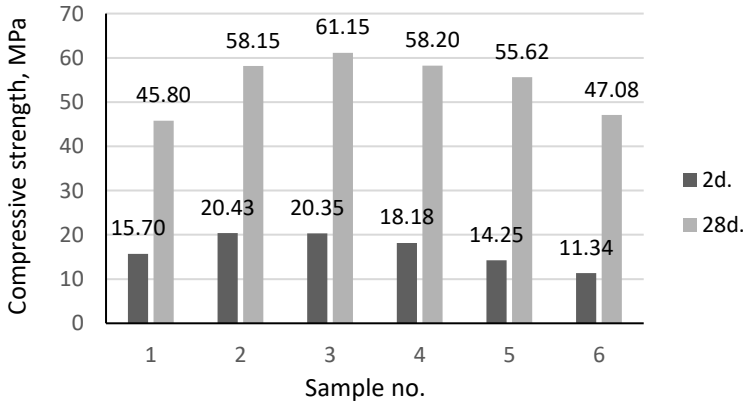

Fig. 1. The compressive strength of the samples hardened for 2 and 28 days

The mixture of ESW and MET acts as a highly effective supplementary cementitious materials, allowing 25% by weight Portland cement to be replaced with this material and improving the compressive strength of cement stone.

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3. BENZO-CARBAZOLE FUNCTIONALIZED BENZOPHENONE HOSTS FOR EFFICIENT RED PHOSPHORESCENT OLEDS USING CO-HOST ENGINEERING

Gintare Krucaite[1]*, Dovydas Blazevicius[1], Raminta Beresneviciute[1], Saulius Grigalevicius[1], Yi-Qi Chao[2], Zih-Ru He[2], Kuan-Yu Su[2], Chih-Hao Chang[2]

[1] Department of Polymer Chemistry and Technology, Kaunas University of Technology, Kaunas, Lithuania
[2] Department of Electrical Engineering, Yuan Ze University, Taiwan
** gintare.krucaite@ktu.lt*

Organic light-emitting diodes (OLED) technology has rapidly evolved into sophisticated multilayer architectures that earned them a spot in commercial flat-panel displays and lighting applications [1–3]. In this work designed and synthesized four new benzophenone-(benzo)carbazole based host materials. The structures of the compounds are shown in the Figure 1.

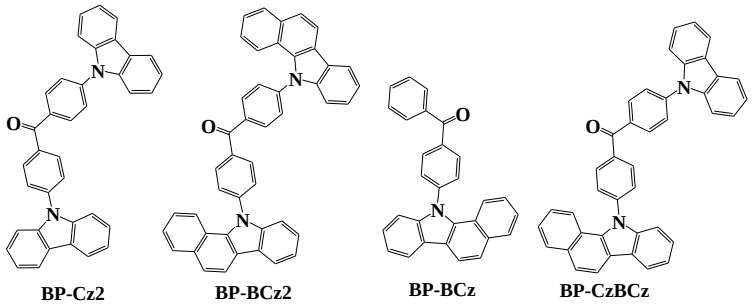

Fig. 1. Structures of target compounds BP-Cz2, BP-BCz2, BP-BCz, BP-CzBCz

All synthesized compounds exhibited excellent thermal stability and a strong tendency to form stable amorphous thin films, with glass transition temperatures exceeding 100 °C for most materials. Photophysical characterization revealed singlet energy levels ranging from 2.90 to 3.61 eV and triplet energy levels between 2.50 and 3.10 eV, corresponding to singlet–triplet energy gaps of 0.35–0.51 eV. These energy characteristics confirm that the benzophenone derivatives provide sufficient exciton confinement for red phosphorescent emitters. Furthermore, charge-transport measurements indicated hole and electron mobilities spanning from 10^{-3} to 10^{-12} $cm^2 V^{-1} s^{-1}$, highlighting the tunability of charge-transport properties through molecular design. The donor-acceptor compounds were evaluated as host materials in red OLED devices. Notably, devices employing a co-host configuration consistently outperformed their single-host counterparts. In particular, the BP-BCz-based co-host system utilizing OLED achieved a maximum external quantum efficiency of 17.9% with a reduced efficiency roll-off at high luminance.

Acknowledgements. This work was supported by the Research Council of Lithuania (Grant No. S-MIP-25-23).

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CONVERTING BIODIESEL WASTE INTO BIOGAS

Ieva Pinkė*, Kiril Kazancev, Violeta Makarevičienė, Eglė Sendžikienė

Agriculture Academy, Vytautas Magnus University, Kaunas, Lithuania
** ieva.pinke@vdu.lt*

The enzymatic process of simultaneous oil extraction and *in situ* interesterification using methyl formate as an acyl receptor can be applied for biodiesel synthesis. This process generates waste (a mixture of rapeseed cake and enzymatic catalyst) that is suitable for energy purposes, such as the production of biogas. Two types of biodiesel waste, consisting of rapeseed cake and Lipozyme TL IM catalyst, were used for biogas production. Waste (W) was obtained via *in situ* interesterification with methyl formate, while waste (WD) was produced similarly but within a mineral diesel medium. Both wastes were separated after processing under optimal laboratory conditions [1,2].

Substrate moisture and volatiles were determined gravimetrically, while C/N content was measured using a CHNS-O analyzer. Biogas production was conducted in an anaerobic bioreactor at 37 ± 1 °C for 30 days. Samples included sewage sludge (WS) mixed with 10, 20, or 30% W or WD, using pure WS as a control. Gas volume and composition were monitored via a milligascounter and GC-TCD analyzer. Interesterification waste is suitable for biogas production either alone or in mixtures with up to 30% sewage sludge (Fig. 1). Pure waste yielded 871.6 ml/g SM over 30 days, nearly double the 488 ml/g DM produced by sewage sludge. However, waste containing diesel residues (WD) showed a lower yield (513.17 ml/g DM) (Fig. 2), likely due to the inhibitory effect of diesel on microbial activity.

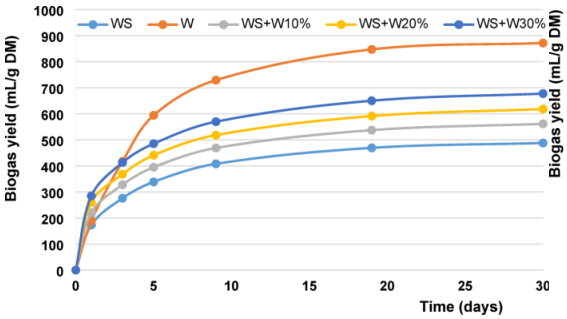

Fig. 1. Biogas yield from biodiesel production waste W and its mixtures with sewage sludge

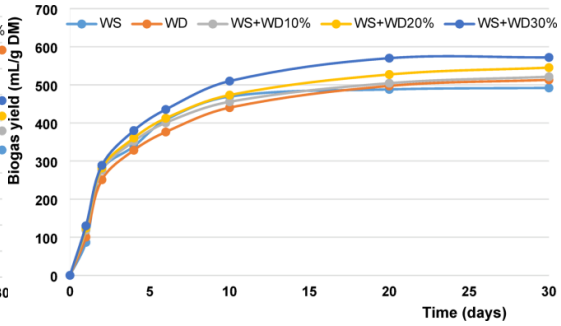

Fig. 2. Biogas yield from biodiesel production waste WD and its mixtures with sewage sludge

In mixtures, biogas yields increased with higher waste concentrations, though this effect was less pronounced for WD. Methane concentrations remained consistent across all samples, ranging from 65.08% to 67.7%, with CO_2 levels between 24% and 28%. Since both yield and composition align with conventional substrates, these wastes are viable for efficient biogas production.

Acknowledgements. The research was funded by a Project MIP-22/59 Synthesis of innovative biodiesel from the Research Council of Lithuania and the Ministry of Education, Science and Sports of the Republic of Lithuania and Research Council of Lithuania (LMTLT) under the Program "University Excellence Initiative" Project "Development of the Bioeconomy Research Centre of Excellence" (BioTEC), agreement No S-A-UEI-23-14.

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RECYCLING AND RECOVERY OF AUTOCLAVED AERATED CONCRETE WASTE

Edita Prichockiene*, Zenonas Valancius

Department of Silicate Technology, Kaunas University of Technology, Kaunas, Lithuania
** edita.rupsyte@ktu.lt*

In the production of autoclaved aerated concrete (AAC) masonry products, about 5% of autoclaved porous mass waste is inevitably obtained during the technological process, the use of which is not resolved. The study aims to investigate the possibility of using AAC waste as an additive in the production of new autoclaved aerated concrete. Such use of waste would solve the ecological problem and help save local raw materials.

All raw materials were weighed and dosed into a mixer in the following sequence: water, ground sand and waste sludge, Portland cement, lime, gypsum and aluminum suspension. The homogeneous mass was poured into a lubricated mold (10×10×10 cm) and stored in it until it acquires the required strength. The sand in the formation mixture was replaced by 6.25, 12.5, and 18.75% of this waste. Curing of the samples was carried out in the autoclave "Parr instruments" (Germany) with a saturated water vapour temperature of 190°C, a pressure of 12.5 bar, an isothermal duration of 11 h. The samples were removed from the molds and dried to a constant mass at 105 ±5 °C after curing. The essence of aerated concrete hardening is that CaO from lime reacts with silica to form 1.13 nm tobermorite. It is known that the minerals of the tobermorite group determine the strength and other properties of such products that are widely used in construction, such as concrete, silicate bricks, gas silicate.

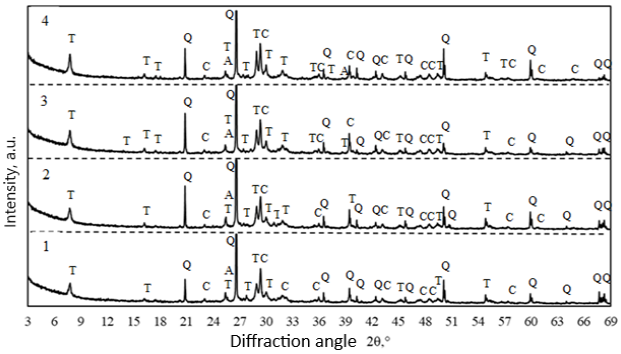

Fig. 1. RSDA curves of samples: 1 – without waste, 2 – with 6.25% waste, 3 – with 12.5% waste, 4 – with 18.75% waste. Here: T – tobermorite 1.13nm; Q – quartz; C – calcite; A – anhydrite

Reviewing the X-ray diffraction analysis, attention was paid to the dependence of the intensity of tobermorite 1.13 nm diffraction peaks on the amount of additive. It has been calculated that replacing a certain part of the sand with hardened waste results in a higher amount of 1.13 nm tobermorite in the resulting aerated concrete, which ensures a higher strength of the sample. Therefore, even 12.5% of AAC waste additive does not impair the properties of the product at all, and the strength even increases to 10%. The results show that solidified waste AAC can be used in the production of blocks. They make it possible to reduce the consumption of natural sand and make production waste-free.

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OPTIMIZING MXENE–TITANIUM INTERFACIAL BONDING FOR DURABLE AND EFFICIENT ELECTROCHEMICAL APPLICATIONS

Mohd Sajid[1]*, Paulius Gaigalas[1], Oleksiy Gogotsi[2], Vaclovas Klimas[1], Simonas Ramanavicius[1]

[1] State Research Institute Center for Physical Sciences and Technology, Department of Electrochemical Material Science, Vilnius, Lithuania
[2] Materials Research Center, Kyiv, Ukraine
** mohd.sajid@ftmc.lt*

The transition toward renewable energy sources is broadly viewed as essential for achieving a sustainable and technologically progressive global landscape. Among the array of clean energy carriers, hydrogen (H_2) stands out as a leading candidate for future fuel systems due to its high energy content and its ability to deliver power without generating carbon-based emissions [1]. With water being plentiful across the planet, it offers an inexhaustible medium for large scale hydrogen extraction. However, developing water splitting technologies that are both efficient and economically feasible remains a major obstacle in modern energy research [2, 3]. Although noble metal electrocatalysts exhibit outstanding catalytic activity for both the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER), their substantial cost limits widespread deployment. This has intensified the search for alternative materials and engineering approaches capable of delivering scalable and cost-effective hydrogen production. Two-dimensional (2D) materials have emerged as compelling options for electrochemical water splitting, and MXenes, in particular, have rapidly gained prominence due to their unique structure and physicochemical properties [4]. Despite this progress, integrating advanced nanomaterials with traditional electrode support to create high performance hybrid systems remains a demanding task. The effectiveness of an electrochemical electrode depends on several interconnected parameters, such as its structural durability, operational stability, ability to ensure efficient water contact, and strong interfacial bonding between active catalysts and the substrate. In this work, cost effective and biocompatible titania (TiO2) was chosen as the base substrate, and a simple, solution-based fabrication route was developed to produce MXene coated Ti electrodes with improved interface strength. To systematically enhance the wettability and adhesion of MXene on the TiO2 surface, four surface engineering techniques like – anodization, plasma treatment, HF etching, and HF–HNO3 activation, were implemented, along with a combined multimodal modification approach. These treatments enabled controlled adjustment of the TiO2 surface chemistry and topography, thereby facilitating stronger MXene attachment. The resulting Ti–MXene hybrid electrodes were then thoroughly assessed for their suitability in electrochemical water splitting applications, demonstrating that tailored interfacial properties significantly contribute to improved catalytic performance.

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DYNAMICS OF CHEMICAL AND PHYSICAL PARAMETERS IN A FERMENTED TEA BEVERAGES DURING PRODUCTION

Marija Vaišvilaitė, Simona Sutkuvienė*, Vaida Andrulevičiūtė

Department of Biochemistry, Faculty of Medicine, Lithuanian University of Health, Kaunas, Lithuania
** simona.sutkuviene@lsmu.lt*

The aim of this study was to analyse the physicochemical parameters of kombucha, an ancient East Asian fermented tea beverage currently gaining global popularity [1], during the production period using different tea samples. It is produced using a symbiotic culture of bacteria and yeasts (SCOBY), resulting in a complex matrix of organic acids, polyphenols, vitamins, and other bioactive compounds [2].

The kombucha beverage was prepared using five types of tea. The drinks were fermented for 9 days, with analyses conducted every 3 days. The pH, titratable acidity, total phenolic content, antioxidant activity, and soluble solids were analyzed. Sensory analysis was conducted on the ninth day of fermentation.

During the analysis period, the pH of the tested beverage decreased significantly, while acetic acid content increased due to the formation of organic acids. Black, green, and cactus blossom green teas showed an increase in total phenolic content during fermentation. Kombucha prepared with oolong tea, exhibited the highest levels of phenolic compounds on the sixth day, followed by a subsequent decrease. Blue “Galaxy” tea showed the lowest levels of these compounds throughout the fermentation period.

Antioxidant activity was influenced by both the type of substrate and fermentation time, exhibiting varying trends across all tea samples. Kombucha prepared with oolong tea demonstrated the most favorable antioxidant activity for consumption (Fig. 1).

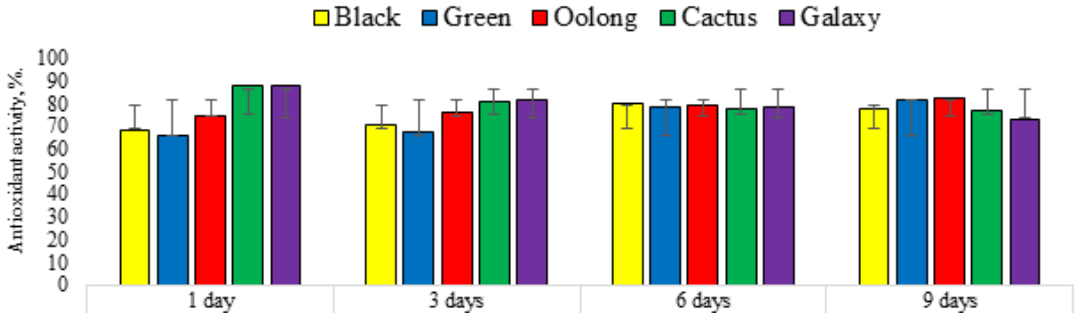

Fig. 1. Antioxidant activity of kombucha prepared using different teas during fermentation

On the ninth day of the study, sensory evaluation was conducted by 10 assessors. The highest scores were assigned to kombucha prepared with blue “Galaxy” tea.

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SUSTAINABLE PROCESSING OF PYROLYSIS OIL USING HYDRODYNAMIC CAVITATION: EXPERIMENTAL STUDY AND MULTIPHASE CFD MODELLING

Aurimas Saltuska*, Mohammad Jakir Hossain Khan, Zilvinas Kryzevicius

Engineering Department, Faculty of Marine Technology and Natural Sciences,
Klaipeda University, Klaipeda, Lithuania
** aurimas.saltuska@ku.lt*

Pyrolysis is considered an alternative route for converting waste into valuable products, including pyrolysis oil. However, the direct use of pyrolysis oil is often restricted by its variable composition, which necessitates further upgrading before practical application in chemical processing and energy-related technologies [1]. Hydrodynamic cavitation has emerged as a promising and sustainable process intensification method due to its relatively simple reactor design, continuous operating capability, scalability potential, and ability to generate intense local pressure fluctuations under comparatively mild overall bulk operating conditions [2].

Table 1. Comparison of iodine number and hydrodynamic indicators, including cycle number (N), momentary cavitation (Cav.), and turbulence intensity (ω), for different orifice plate configurations at 5 bar.

Sample	**P1**	**P5**	**P10**	**P15**	**P21**
Iodine	44.42	25.38	19.33	14.59	10.39
N	280.83	301.13	313.37	312.33	318.44
Cav.	1.12	1.70	3.42	3.50	2.52
ω	6394	6817	7084	6356	7613

Five orifice plates were designed and manufactured in this study, differing only in the number of holes, while all other geometric parameters were kept constant to ensure an objective comparison. Experimental conditions were maintained by varying only the plate configuration and operating pressure at 3, 4, and 5 bar. To support process interpretation, multiphase CFD modelling of a two-liquid flow system was performed. This approach enabled analysis of velocity fields, pressure variations, momentary cavitation (Cav.), turbulence intensity (ω), and overall flow behavior inside the reactor [3]. Representative results for the 5-bar operating pressure are presented in Table 1.

The combined experimental and numerical approach was used to evaluate the influence of plate geometry and operating pressure on pyrolysis oil treatment. The results indicate that both orifice design and operating pressure significantly affect the hydrodynamic environment in the cavitation zone and, consequently, the suitability of the reactor for pyrolysis oil processing. Overall, hydrodynamic cavitation is shown to be a promising low-complexity approach for sustainable preliminary treatment of pyrolysis oil and a useful basis for further reactor development using CFD and experimental data.

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WHEAT GLUTEN FIBROUS SCAFFOLDS FOR CULTIVATED MEAT APPLICATIONS

Eidvylė Gasiulytė*, Ingrida Pauliukaitytė, Edvinas Krugly, Darius Čiužas

Faculty of Chemical Technology, Kaunas University of Technology, Kaunas, Lithuania
** e.gasiulyte@ktu.lt*

The increasing global demand for meat presents significant ethical, environmental, and food safety challenges, accelerating the development of cultivated meat technologies [1]. A critical challenge in the engineering of *in vitro* meat analogues is the selection of appropriate biomaterials capable of replicating the native muscle tissue structure. Plant-derived proteins are promising candidates due to their sustainability, cost-effectiveness, biocompatibility, and biodegradability [2]. Wheat gluten is a viscoelastic protein capable of forming interconnected network structures suitable for fibrous scaffolds fabrication [3].

Wheat gluten-based fibrous scaffolds for meat tissue structuring were fabricated using solution electrospinning. Solutions were prepared in acidified water–ethanol or acetic acid–ethanol systems at varying ratios, followed by the addition of poly(ethylene oxide), glucose, and glycerol as functional additives.

Solvent composition strongly influenced solution electrical conductivity, rheological properties, and electrospinning stability. Fiber formation ranged from droplet formation to continuous microfibers (Fig. 1). SEM analysis confirmed the formation of fibrous scaffolds with average fiber diameters ranging from 0.66 µm to 3.85 µm.

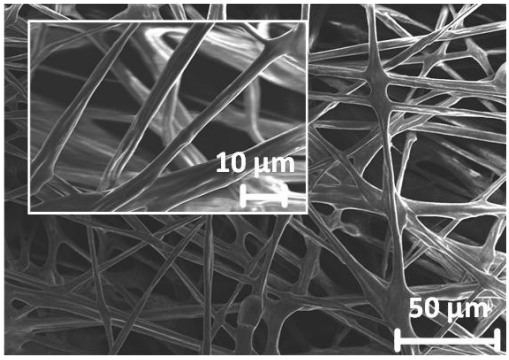

Fig. 1. SEM image of wheat gluten scaffold prepared in an acidified water:ethanol (3:7) solvent system

The study demonstrates that food-grade solvent systems enable the fabrication of edible wheat gluten microfibrous scaffolds. Control of solution composition allows tuning of physicochemical properties and fiber diameter, making electrospinning as a promising approach for cultivated meat applications.

Acknowledgements. This work was supported by Research Council of Lithuania “Edible Fibrous Polymer Scaffolds for Meat Cultivation” (Grant No. S-MIP-25-61).

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EFFECT OF BORON CO-DOPING ON OPTICAL EMISSION IN GARNETS

Greta Inkrataitė[1]*, Jan-Niklas Keil[2], Thomas Jüstel[2], Ramūnas Skaudžius[1]

[1]Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Vilnius, Lithuania
[2]Department of Chemical Engineering, Münster University of Applied Sciences, Steinfurt, Germany
** greta.inkrataite@chgf.vu.lt*

In order to convert high-energy radiation, such as gamma or X-rays, into visible light scintillating materials are needed. Over the years many different candidates to fit the requirements were examined. However, compounds with garnet structures have attracted a particularly large amount of attention. Praseodymium doped lutetium and gadolinium aluminum garnets have high density, high thermal stability, rather efficient luminescence processes, and thus high quantum efficiency which are needed for a good scintillator [1]. However, further optimization and improvement are still required especially w.r.t. a reduced decay time. The duration of the luminescence decay is important because if it is very short then the more signals can be measured within a defined timeframe, resulting in a better resolved and higher quality image, for example in CT or PET devices. One way to improve materials properties is to doping the aforementioned compounds with different elements. As such, by doping we could potentially be able to improve key aforementioned parameters: emission intensity, quantum efficiency and decay times [2,3]. One of these elements is boron. Primarily, it can be used as a flux, and also B^{3+} ion has a suitable neutron capture cross section and can also help absorb gamma radiation [4]. However, garnets can be doped with larger amounts of other elements. In this case, we replaced some of the aluminum with scandium. Lutetium aluminum garnets and gadolinium aluminum garnets doped with Pr^{3+} and B^{3+} were obtained as a result.

In the present work, the effect of boron on the various characteristic of the LuAG and GdAG doped by praseodymium is investigated. Garnets doped with different amounts of boron were synthesized by the aqueous sol-gel method. The phase purity of the samples was analyzed by means of X-ray diffraction (XRD). The morphology of the compounds was evaluated by using scanning electron microscopy (SEM). Photoluminescence properties such as emission and excitation spectra, decay curves, quantum efficiency and temperature dependency of the emission and excitation spectra have been investigated. Radioluminescence was also measured in order to determine the scintillation properties of the samples. The positive impact of boron addition into the garnet structure on the luminescence properties will be discussed in detail

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MODULATING MAGNETIC PROPERTIES OF $CoFe_2O_4$ NANOPARTICLES WITH AMINO ACID-BASED SURFACTANTS

Aswathi Raveendran*, Germante Paulikaite, Audrius Drabavicius, Vidas Pakstas, Kestutis Mazeika, Aldona Balciunaite, Martynas Talaikis, Agne Mikalauskaite, Simonas Ramanavicius

Center for Physical Sciences and Technology, Department of Electrochemical Materials Research, Vilnius, Lithuania
** aswathi.raveendran@ftmc.lt*

The unique, size-controllable physicochemical and magnetic characteristics of magnetic nanoparticles have positioned them as vital components in fields ranging from biomedicine and photocatalysis to data storage [1,2,6]. Cobalt ferrite ($CoFe_2O_4$) stands out among these materials due to its exceptional chemical durability, mechanical robustness, and high magneto crystalline anisotropy. Nevertheless, the functional efficacy of $CoFe_2O_4$ depends strictly on its size and shape, which are determined by the synthesis environment [3–5]. A common challenge is that these nanoparticles tend to clump together (agglomerate) due to their high surface energy and magnetic attraction. To solve this, surfactants or capping agents are used to create repulsive forces – either electrostatic or steric – that keep the particles separate and stable [6].

In this research, $CoFe_2O_4$ nanoparticles were fabricated using a hydrothermal co-precipitation approach, evaluating the effects of amino acids as stabilizing capping agents [1]. A comprehensive characterization of the resulting crystallographic structures, magnetic responses, and morphological features was conducted using TEM, XRD, VSM, UV spectrometry, and BET analysis. The results demonstrate that surface-modified CoFe2O4 nanoparticles exhibit enhanced stability and performance, establishing them as highly effective, magnetically recoverable catalysts and adsorbents for advanced wastewater treatment applications.

Acknowledgements. This project received funding from the Research Council of Lithuania (LMTLT), agreement No S-MIP-24-14.

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SYNTHESIS OF 3-[1-(2,4-DIFLUOROPHENYL)THIOUREIDO]PROPANOIC ACID AND ITS DERIVATIVES

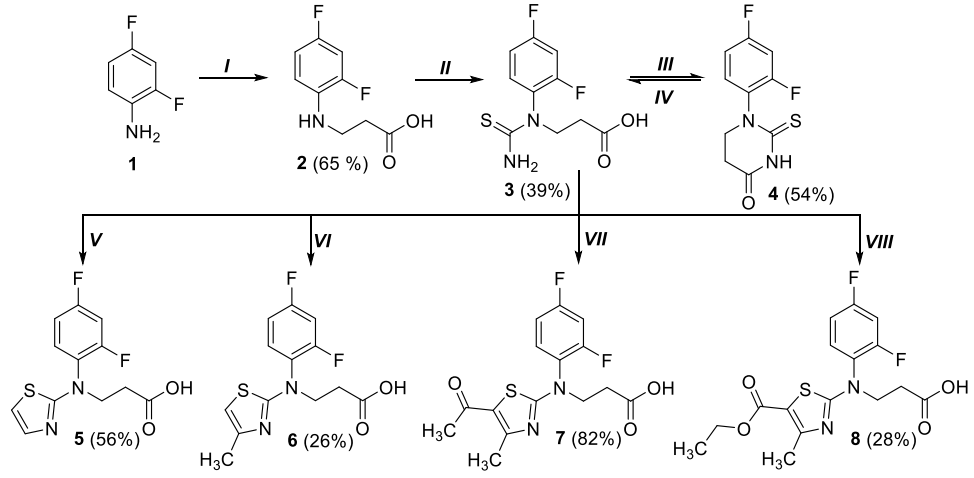
Guoda Pranaitytė*, Birutė Grybaitė, Vytautas Mickevičius, Marcelina Mažonytė

Department of Organic Chemistry, Kaunas University of Technology, Lithuania

** guoda.pranaityte@ktu.lt*

Thioureido acids are used in organic chemistry as intermediates in the synthesis of molecules with heterocyclic moieties such as thiazoles [1]. Five-membered thiazole pharmacophore is frequently occurring in FDA-approved drugs, such as *Fentiazac*, *Meloxicam* or *Dasatinib* [2, 3].

Commonly, reactions of *β*-amino acids with alkali metals' thiocyanates in the acidic medium result in the formation of 2-thioxotetrahydropyrimidine-4(1H)-ones. First, *β*-alanine 2 was synthesized from amine 1 and acrylic acid. The condensation of *β*-alanine 2 with potassium thiocyanate in acetic acid was carried out under reflux for 24 h. The formed intermediate – thioureido acid 3 was cyclized *in situ* with hydrochloric acid to the more stable and acid-resistant heterocycle - 1-(2,4-difluorophenyl)-2-thioxotetrahydropyrimidine-4(1H)-one (4). The target thioureido acid 3 was obtained by decyclization of compound 4 in alkaline medium. One of the most convenient methods for the preparation of thiazoles is the *Hantzsch* synthesis, i.e. the condensation of *β*-halocarbonyl derivatives with thioamides or thiocarbamides. This method was used to synthesize compounds 5–8 containing an aminothiazole ring.



Reagents and conditions: (***I***) acrylic acid, Δ, toluene, 24 h; (***II***) KSCN, Δ, CH_3COOH, 24 h; (***III***) H^+, pH 1, Δ, 1 h; (***IV***) OH^-, Δ; (***V***) 50% chloroacetaldehyde, Δ, 10% Na_2CO_3, 24 h; (***VI***) chloroacetone, Δ, 10% Na_2CO_3, 24 h; (***VII***) 1) 3-chloro-2,4-pentandione, Δ, acetone, 24 h, 2) 5% CH_3COONa, Δ; (***VIII***) ethyl-2-chloro-acetoacetate, Δ, 5% CH_3COONa, 1 h.

Fig. 1. Synthesis of 3-[1-(2,4-difluorophenyl)thioureido)propanoic acid and its derivatives containing a thiazole moiety

The structure of the synthesized compounds has been proven by ^1H NMR, ^{13}C NMR and other spectroscopic methods. These compounds are currently being investigated for their potential anticancer activity.

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SYNTHESIS AND APPLICATION OF BIFUNCTIONAL ORGANIC MATERIALS FOR PASSIVATING PEROVSKITE COMPOSITIONS IN PEROVSKITE SOLAR CELLS

Justina Mikučiūnaitė*, Kasparas Rakštys

Department of Organic Chemistry, Faculty of Chemical Technology, Kaunas University of Technology, Kaunas, Lithuania

** justina.mikuciunaite@ktu.lt*

As a rapidly evolving technology, perovskite solar cells have attracted significant attention in the scientific community, with efficiencies surpassing silicon-based solar cells [1]. Their low-cost fabrication and mechanical flexibility boost their potential for scalable applications. Despite advances in photovoltaic technologies, high efficiency and long-term stability remain challenging. Perovskite materials are sensitive to environmental stressors and susceptible to defect states during synthesis. These defects act as non-radiative recombination centres, limiting both performance and stability. To address this, surface passivation strategies—especially those using organic salts—are used to reduce defect density and improve efficiency [2].

Building on these advancements, previously conducted research found that the isothiouronium functional group interacts well with the perovskite layer and reduces various defects. To further improve the interface between the perovskite and hole-transport materials, an additional functional group was incorporated to interact with the charge-transporting layer. Accordingly, a series of new organic materials was synthesised in a single step by introducing isothiouronium moieties functionalised with phosphonic or carboxylic acids. These acids serve as anchoring groups that interact with the ITO contact material [3]. This enables fast charge transport and improves the overall performance of perovskite solar cells. Passivating agents were used to passivate the perovskite bottom layer in inverted-structure devices.

In the context of these developments, bifunctional passivating agents were compared, and the effect of the resulting compounds on perovskite solar cells was evaluated. Passivated perovskite solar cells with the highest reported efficiencies were subsequently sent to an independent photovoltaic calibration laboratory for certified measurements, which yielded 26.8% for a 0.05 cm^2 device and 25.2% for a 1.03 cm^2 device.

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EXPLORING CLASSICAL AND ELECTROCHEMICAL APPROACHES TO SUBSTITUTED CARBOXYLIC ACIDS

Aida Šermukšnytė[1]*, Kristina Kantminienė[1], Jaime A. S. Coelho[2], Ingrida Tumosienė[1]

[1] Kaunas University of Technology, Kaunas, Lithuania
[2] University of Lisbon, Lisbon, Portugal
** aida.sermuksnyte@ktu.lt*

The synthesis of substituted carboxylic acids is fundamental in organic and medicinal chemistry because of their usage in pharmaceuticals and functional materials. 2-Aminopyridines are a convenient starting point for derivatization, as their amino group and pyridine core can undergo diverse transformations to yield new bioactive compounds [1]. In this work, the functionalization of novel carboxylic acid derivatives using both classical chemical synthesis and preliminary electrosynthesis is presented.

In the classical approach, 2-amino-5-chloropyridine was condensed with itaconic acid to form a corresponding oxopyrrolidinecarboxylic acid [2]. This intermediate was coupled with various amines using HBTU and TEA to afford the target derivatives. The structures of the novel compounds were confirmed by ^{1}H and ^{13}C NMR spectroscopy as well as mass spectrometry.

Electrochemical Shono-oxidation was performed on the oxopyrrolidinecarboxylic acid to form a methoxy-substituted intermediate [3]. The synthesis was carried out by using graphite (anode) and platinum (cathode) electrodes in methanol with supporting electrolytes ($^{n}Bu_4NPF_6$ or $LiClO_4$) under controlled current or controlled potential. Cyclic voltammetry-guided optimization of electrochemical reaction conditions revealed the redox behavior of the starting material. Preliminary analyses indicated the formation of the desired derivative, but the isolation of the pure product was challenging due to the presence of unreacted starting compounds.

Overall, this work highlights the efficiency of a classical synthesis of the pyrrolidinecarboxylic acid scaffold from itaconic acid, while demonstrating the potential of electrosynthesis to generate a structurally modified intermediate via anodic oxidation. Electrochemical approaches like Shono-oxidation enable access to methoxylated derivatives, expanding the diversity of novel compounds. Future work will aim to improve product isolation and expand the range of derivatives.

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A DIVERGENT ROUTE TO HSP90 INHIBITORS FEATURING RESORCINOL AND THIADIAZOLE PHARMACOPHORES

Vilius Petraška*, Ieva Žutautė

Faculty of Chemistry and Geosciences, Vilnius University, Lithuania
vilius.petraska@chgf.vu.lt

Hsp90 (Heat Shock Protein 90) is a molecular chaperone that stabilizes proteins under stress conditions, facilitates their degradation, and ensures proper protein folding. Cancer cells contain elevated levels of this protein, and studies have shown that Hsp90 plays a crucial part in many aspects of tumor progression [1]. As a result, Hsp90 is being thoroughly investigated as a target for anticancer treatments [2].

Analysis of natural compounds resulted in the identification of resorcinol (1) as an essential structural motif for binding to the Hsp90 N-terminal domain. This region contains the ATP-binding pocket, which is vital for the protein's function. While many different compounds have been examined, the 4th position of the resorcinol ring is comparatively underexplored.

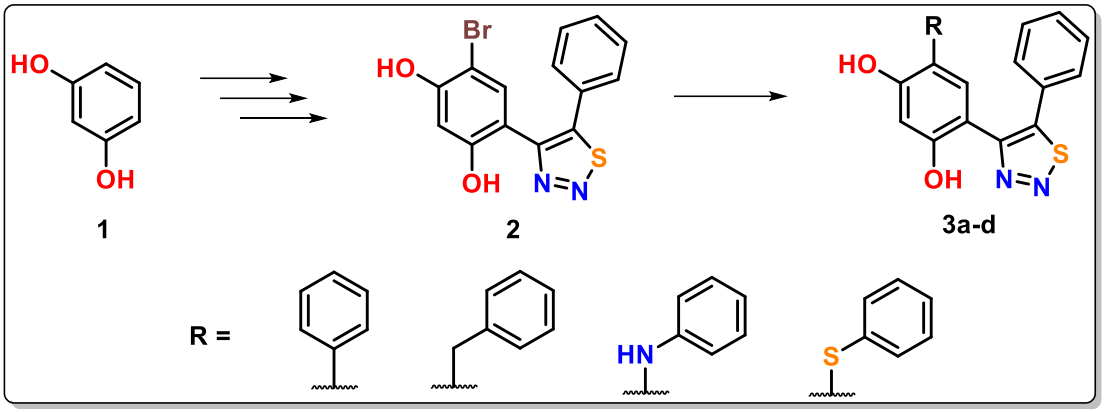

Fig. 1. Resorcinol 1 and target structures 3a-d

The aim of this work was to synthesize a range of Hsp90 inhibitors with hydrophobic substituents at the 4th position of the resorcinol fragment. Utilizing palladium chemistry, four different types of compounds (3a-d) were obtained using Buchwald-Hartwig and Suzuki coupling reaction conditions. The presentation will cover the divergent synthesis process, its challenges, and results.

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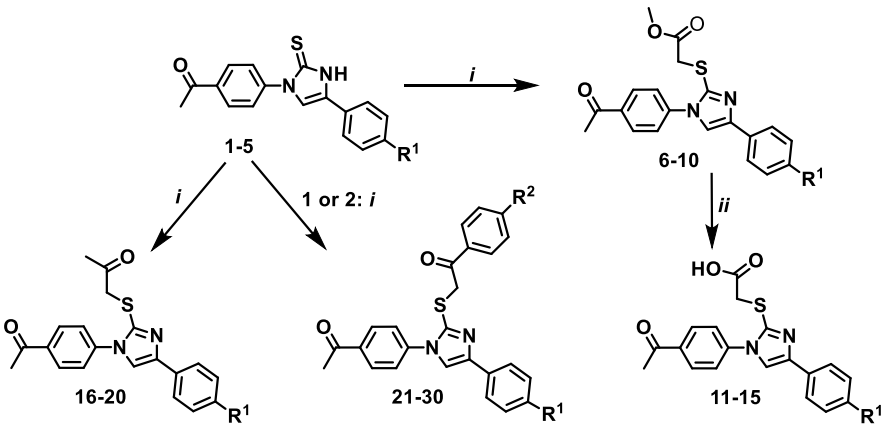
SYNTHESIS AND PHARMACOLOGICAL EVALUATION OF IMIDAZOLE-2-THIONE DERIVATIVES

Božena Golcienė[1]*, Birutė Sapijanskaitė-Banevič[1], Anoop Kallingal[2], Natalia Maciejewska[2], Vytautas Mickevičius[1]

[1] Kaunas University of Technology, Department of Organic Chemistry, Kaunas, Lithuania
[2] Gdansk University of Technology Department of Pharmaceutical Technology and Biochemistry, Gdansk, Poland
** bozena.golciene@ktu.lt*

Imidazole-based structures are widely valued in drug development due to their biological activity and ease of synthesis. In this study, a series of *S*-substituted imidazole-2-thione derivatives was designed and evaluated, with 2-{[1-(4-acetylphenyl)-4-(4-chlorophenyl)-1H-imidazol-2-yl]thio}-1-(4-chlorophenyl)ethan-1-one (24) emerging as the most promising candidate (Fig. 1).



Reagents and conditions: *i* methyl 2-bromoacetate (for 6-10), 1-chloropropan-2-one (for 16-20) or the corresponding bromoacetophenone (for 21-30), MeOH, anhydrous K_2CO_3, Δ, 1-2 h; *ii* 18.5 % HCl, Δ, 1 h. 1, 6, 11, 16 R^1 = H, 2, 7, 12, 17 R^1 = Cl, 3, 8, 13, 18 R^1 = OH, 4, 9, 14, 19 R^1 = F, 5, 10, 15, 20 $R_1 = NO_2$; 21 $R^1 = R^2$ = H, 22 R^1 = Cl, R^2 = H, 23 R^1 = H, R^2 = Cl, **24 $R^1 = R^2$ = Cl**, 25 R^1 = H, R^2 = F, 26 R^1 = Cl, R^2 = F, 27 R^1 = H, R^2 = CF3, 28 R^1 = Cl, $R^2 = CF_3$, 29 R^1 = H, $R^2 = OCF_3$, 30 R^1 = Cl, $R^2 = OCF_3$.

Fig. 1. Synthesis of imidazole-2-thione derivatives 6-30

It demonstrated strong cytotoxic effects against lung, cervical, and colorectal cancer cell lines, exhibiting submicromolar IC_{50} values. Mechanistic studies indicated that its activity involves induction of G1 phase cell cycle arrest, activation of caspase-mediated apoptosis, and increased levels of phosphorylated γH2AX. Notably, compound 24 significantly reduced migration and invasion of A-549 cells in both 2D and 3D models. Enzymatic assays confirmed that it can directly inhibit MMP-9 activity. *In vivo* experiments using the CAM model showed that compound 24 effectively limited tumor growth and vascular dissemination without observable toxicity. Overall, these findings suggest that compound 24 is a strong candidate for anticancer therapy, combining cytotoxic and anti-metastatic effects and warranting further preclinical evaluation.

HIGH-PERFORMANCE OLED HOST MATERIALS: PHOTOPHYSICAL PROPERTIES AND DEVICE OPTIMIZATION OF CARBAZOLE-BENZOCARBAZOLE DERIVATIVES

Daiva Tavgenienė[1]*, Dovydas Blazevicius[1], Inesa Sasnauskaitė[1], Saulius Grigalevicius[1], Chi-Hao Huang[2], Yu-Hsuan Chen[2], Chih-Hao Chang[2]

[1] Kaunas University of Technology, Kaunas, Lithuania
[2] Yuan Ze University, Taoyuan, Taiwan
* *daiva.tavgeniene@ktu.lt*

Organic light-emitting diodes (OLEDs) have been at the forefront of advancements in personal electronics and lighting applications in recent years. To further enhance device efficiency, the development of new host materials for phosphorescent and TADF emitters is essential. Motivated by this need, we designed and synthesized carbazole-benzo[*a*]carbazole-based compounds with controlled alkyl substitution as hole-transporting hosts, incorporating ethyl (eCzBCz) or butyl (bCzBCz) chains to improve film-forming properties for yellow TADF and red phosphorescent OLEDs. These new materials exhibited high thermal stability ($T_d \approx 350$ °C) and the ability to form amorphous layers, with eCzBCz demonstrating a particularly high T_g level of 107 °C. Photophysical analyses reveal distinct fluorescence and phosphorescence spectra, with respective singlet (triplet) energy gaps of 3.47 eV (2.53 eV) and 3.47 eV (2.50 eV). Due to their strong hole transport but weak electron transport capabilities, a co-host system incorporating CN-T2T was introduced to enhance negative charge transport. OLED devices using these materials demonstrated improved charge balance, higher efficiency, and reduced efficiency roll-off. Devices with blended hosts exhibited superior external quantum efficiency (EQE) exceeding 20 % and stable color emissions. Additionally, the lifetime tests confirmed the higher stability of eCzBCz-based devices under high electric fields, highlighting their potential for high-performance OLED applications.

Acknowledgements. This work was supported by the Research Council of Lithuania (Grant No. S-LLT-25-2).

3,6-BIS(DIPHENYLAMINO)CARBAZOLE-SUBSTITUTED CYANOPYRIDINES FOR EFFICIENT GREEN AND NIR TADF EMISSION

Dovydas Blazevicius[1]*, Daiva Tavgeniene[1], Gintare Krucaite[1], Raminta Beresneviciute[1], Saulius Grigalevicius[1], Szu-Jung Wang[2], Zhi-Yu Yuan[2], Chen-Hao Chang[2], Chih-Hao Chang[2]

[1] Department of Polymer Chemistry and Technology, Kaunas University of Technology, Kaunas, Lithuania
[2] Department of Electrical Engineering, Yuan Ze University, Chung-Li, Taiwan
** dovydas.blazevicius@ktu.lt*

This study investigates two structurally analogous green thermally activated delayed fluorescence (TADF) emitters, 5Py2CN-CzDPA and 2Py4CN-CzDPA, with a focus on how subtle positional modifications of the acceptor unit influence photophysical behavior and device performance (Fig. 1, 2). Thin-film characterization reveals that both emitters exhibit high photoluminescence quantum yields, small singlet-triplet energy gaps (ΔE_{ST} ≈ 0.10-0.19 eV), and pronounced delayed fluorescence [1], confirming efficient reverse intersystem crossing [2]. Despite comparable intrinsic photophysical properties, significant differences arise in device performance. OLEDs based on 5Py2CN-CzDPA achieve a maximum external quantum efficiency (EQE) of 17.9%, substantially outperforming 2Py4CN-CzDPA-based devices (8.4%), primarily due to improved radiative efficiency and carrier transport balance.

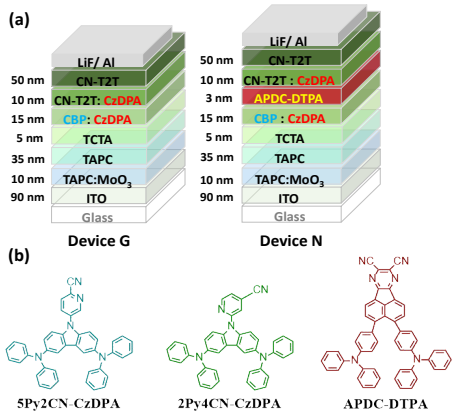


Fig. 1. Schematic structures of the fabricated OLEDs with different emitters (a); structural drawings of the emitters used in OLEDs (b)

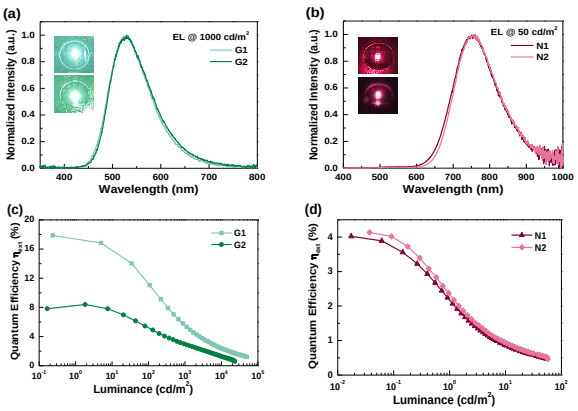


Fig. 2. Normalized EL spectra (a); normalized EL spectra (b); EQE vs. luminance for devices G1 and G2 (c); EQE vs. luminance for devices N1 and N2 (d)

These emitters were further employed as sensitizers to drive near-infrared (NIR) emission using APDC-DTPA as emitter, enabling efficient exciton generation and energy transfer [3], achieving NIR emission at 760.5 nm with a high EQE of 4.13%, among the best reported in this spectral region. Overall, this work demonstrates that minor structural variations can lead to disproportionate impacts on device efficiency and highlights the effectiveness of TADF-sensitized strategies for advancing high-performance NIR OLED technologies.

Acknowledgements. The authors gratefully acknowledge the funding support from the Research Council of Lithuania (Grant No. S-LLT-25-2).

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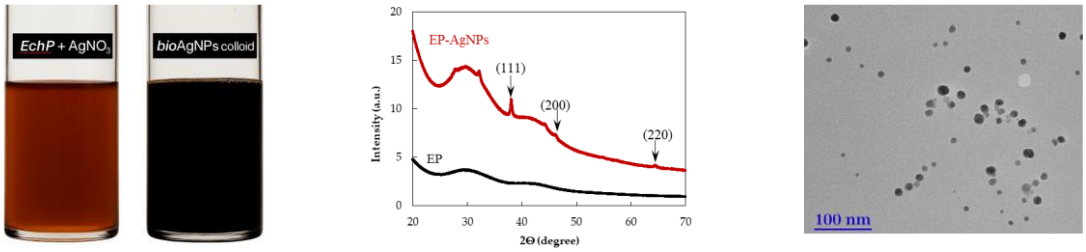
BIOSYNTHESIS OF SILVER NANOPARTICLES VIA *ECHINACEA PURPUREA* EXTRACT: MECHANISM AND FUNCTIONAL EVALUATION

Akvilė Andziukevičiūtė-Jankūnienė[1]*, Erika Adomavičiūtė[1],
Virgilijus Valeika[2], Virginija Jankauskaitė[1]

[1] Department of Production Engineering, Kaunas University of Technology, 51424 Kaunas, Lithuania;
[2] Department of Polymer Chemistry and Technology, Kaunas University of Technology, 51424 Kaunas, Lithuania
** akvile.andziukeviciute-jankuniene@ktu.edu*

Echinacea purpurea (*EchP*) exhibits bioactive properties relevant for biomedical applications, but its antimicrobial efficacy alone is often insufficient against resistant bacteria. Silver nanoparticles (AgNPs) can overcome this limitation by providing enhanced and broad-spectrum antibacterial activity. Accordingly, *EchP* is well-suited for the green synthesis of AgNPs due to its high content of polyphenols and other redox-active phytochemicals that facilitate Ag^+ reduction and nanoparticle stabilization. Therefore, biogenic AgNPs (bioAgNPs) represent a promising antibiotic-free approach to overcoming antimicrobial resistance through broad-spectrum activity [1,2]. This study aimed to investigate the mechanism of bioAgNPs synthesis using *EchP* aqueous extract and to evaluate the properties of the resulting nanoparticles. BioAgNPs were synthesized by reducing Ag^+ ions from $AgNO_3$ in *EchP* extract, and their formation was confirmed by CIELAB analysis (Fig. 1 a) and UV-Vis. FTIR confirmed the involvement of –OH, C=O, and $–NH_2$ groups in bioreduction and capping of nanoparticles, while XRD verified the formation of crystalline, face-centered cubic AgNPs (Fig. 1b). TEM images revealed predominantly spherical, polydisperse particles with an average diameter of ~20.5 nm (Fig. 1c). The synthesized bioAgNPs exhibited enhanced antibacterial activity compared to the native extract, with inhibition zones increasing by 25–30%, particularly against Gram-positive bacteria.



a b c

Fig. 1. *EchP* and bioAgNPs analysis: a – change in colour, b - XRD curves, c – TEM image [2]

The synthesized silver nanoparticles were well-dispersed and effectively stabilized by *EchP* extract. Antibacterial activity makes bioAgNPs suitable for biomedical applications.

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INFLUENCE OF ALKALINE METAL IONS ON THE FILLING OF ALUMINA PORES WITH Cu VIA AC DEPOSITION

Vaclovas Klimas*, Katsiaryna Chernyakova, Tomas Sabirovas, Martynas Talaikis, Jūratė Vaičiūnienė, Arūnas Jagminas

State Research Institute Center for Physical Sciences and Technology, LT-10257 Vilnius, Lithuania
** vaclovas.klimas@ftmc.lt*

In the case of AC treatment, the barrier layer acts like a couple of *n*- and *p*-semiconductors rectifying current like a diode: the deposition occurs at the cathodic half cycle while at the anodic cycle, the damaged points are repaired [1]. The most harmful ions in the electrochemical coloring solutions of porous alumina films are Na^+ and K^+. The intensity of film color obtained by AC treatment in the acidic copper sulfate solution remained similar if alkaline metal ion concentration (c_{Na+} and c_{K+}) did not exceed 20–25 mmol L^{-1}. With further c_{Na+} and c_{K+} increase, the color of films faded (Fig. 1a), and the amount of deposited Cu^0 for the same deposition conditions decreased drastically (Fig. 1b, plots 1 and 2). At the same time, the amount of evolved gas, most likely H_2, increased drastically, attaining ca. 100 µL cm^{-2} during 5 min of the AC treatment at U_{eff} = 10 V (Fig. 1b, plots 4 and 3) instead of ca. 2 µL cm^{-2} characteristic to AC treatment in pure Cu^{2+}/Mg^{2+} solutions.

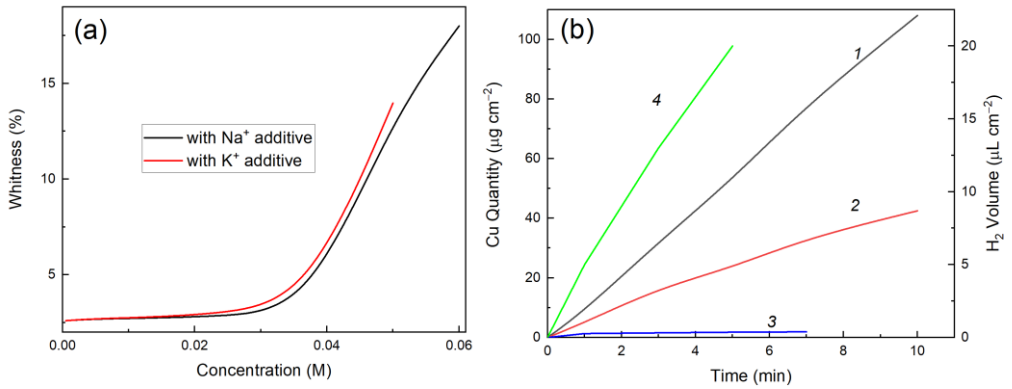

Fig. 1. The color intensity fade of sulfuric acid AAO film after 5 min AC treatment at U_{eff} = 10 V depending on the Na^+ and K^+ concentration in the electrolyte containing 0.1 mol L^{-1} $CuSO_4$ + 0.1 mol L^{-1} $MgSO_4$ + H_2SO_4 to pH 1.5 (a). The quantity of Cu inserted (1, 2) and gases evolved (3, 4) in the AAO pores via AC treatment time at U_{eff} = 10 V in the pure electrolyte (0.1 mol L^{-1} $CuSO_4$ + 0.1 mol L^{-1} $MgSO_4$+H_2SO_4 to pH 1.5) (1, 3) and the same electrolyte containing 0.025 mol L^{-1} Na_2SO_4 (2, 4). Al 99.5 % purity (b)

We established that, in contrast to the detrimental influence of Na^+ and K^+ ions on the dissolution of the alumina barrier layer in some pores during AC deposition, Li^+ ions do not cause significant breakdown, hydrogen evolution, or disruption of NW uniformity growth. This effect was attributed to the formation of small, insoluble $LiAlO_2$ (“corks”) in the channels of the alumina barrier layer. EIS, Raman and FTIR spectroscopy, and SEM were employed. The quantitative evolution of the deposited metal inside the alumina pores under the designed AC conditions was performed using ICP-OE spectrometry.

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INFLUENCE OF WASHED AND HYDROTHERMALLY TREATED BYPASS DUST ON THE HYDRATION OF PORTLAND CEMENT

Brigita Savickaite*, Rimvydas Kaminskas, Anatolijus Eisinas

Kaunas University of Technology, Kaunas, Lithuania
** brigita.savickaite@ktu.lt*

This work investigates the influence of washed and hydrothermally treated Portland cement production bypass dust (BP) on the hydration of Portland cement. The chemical compositions of the dust are as follows (wt. %): SiO_2 – 9.29; Al_2O_3 – 2.76; Fe_2O_3 – 2.15; CaO – 47.70; MgO – 1.68; K_2O – 15.30; Na_2O – 0.50; SO_3 – 6.90; Cl – 10.30; P_2O_5 – 0.08; TiO_2 – 0.19; other – 3.15. For hydrothermal synthesis, washed BD was mixed with quartz to achieve the CaO/SiO_2 (C/S) molar ratios of 1.167. The autoclave operated at a saturated steam temperature of 200 °C, with isothermal hold durations ranging from 2 to 24 hours. It was estimated that after 2 hours of synthesis, in the samples dominate unreacted SiO_2 and calcite together with the beginning of tobermorite formation. The overall trend does not change after 4 hours of hydrothermal treatment. After 8 and 24 hours of synthesis, the development of scawtite is observed and it increases along with a more noticeable amount of tobermorite. For the next investigation, samples after 24 h of synthesis (BP24) were chosen. The results of the investigation show that incorporation of the BP24 additive results in a substantial increase in the water required to achieve normal consistency in cement pastes. Additionally, all samples with this additive demonstrate a modest extension in setting times compared to pure Portland cement paste (OPC). Isothermal calorimetry tests (Fig. 1) were performed on a pure Portland cement sample, as well as samples in which 5% to 15% by weight of cement was substituted with the BP24 additive.

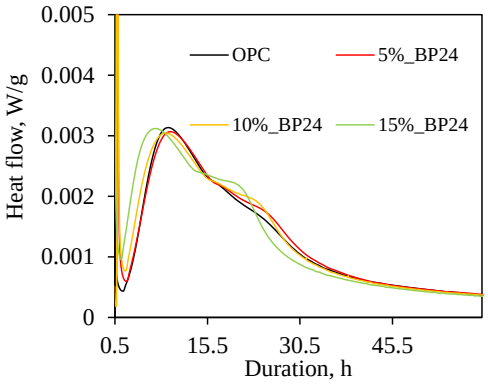

Fig. 1. Calorimetric curves of heat flow of Portland cement samples with different amount of additive

In summary of the results of the research, it can be stated that the additive investigated accelerates the early hydration of Portland cement by promoting both the hydration of calcium silicates and the reaction of the aluminate phase. Furthermore, the compressive strength test of the samples with different amounts of BP24 additive was performed. It was estimated that up to 7.5 wt. % of Portland cement can be replaced with BP24 additive while maintaining the same strength class of the samples.

INFLUENCE OF NICKEL ELECTROPLATING BATH COMPOSITION ON ANODIZED ALUMINIUM COLOURING

Paulius Gaigalas*, Vaclovas Klimas, Tomas Sabirovas, Martynas Talaikis, Jūratė Vaičiūnienė, Arūnas Jagminas

State Research Institute Center for Physical Sciences and Technology, Vilnius, Lithuania
** paulius.gaigalas@ftmc.lt*

Colouring of anodized aluminium via Alternating current (AC) filling of alumina films is an established technique for producing durable coloured finishes, useful for architectural panels and structural components. Besides the aesthetic applications, AC colouring can also be employed to change various physical properties of anodized aluminium films, depending on the species deposited into the pores of film [1–2].

In this study Ni electrodeposition baths of different pH and various concentrations of $MgSO_4$ additive were used in a range of U_{eff} in order to investigate the properties of Ni electrodeposition and determine the conditions for most effective electrocolouring.

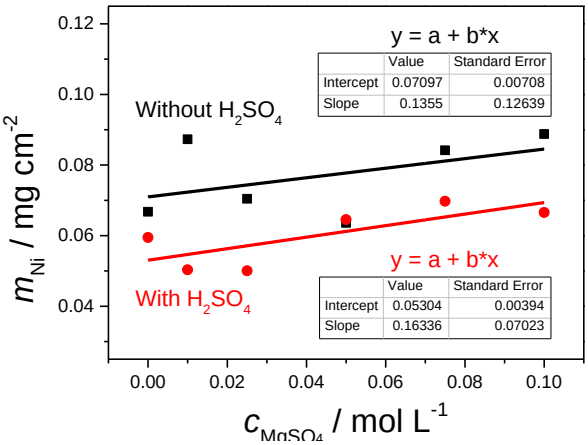

Fig. 1. Influence of $MgSO_4$ concentration on the quantity of electrodeposited Ni without (pH 4.6; black curve)/with additional 1.25 mM H_2SO_4 (pH 3.05; red curve)

It was determined that a noticeable change in colour of anodized aluminium samples occurs at U_{eff} 12 V for most baths in which substantial electrodeposition of Ni was noticeable (pH 3.05 – 4.7), below 9 V or above 13 V the samples appear to have a brown-gray colour and around 15 V first signs of a barrier layer breakdown are observed. When electrodeposition bath pH was below 3.05 or above 4.7, no meaningful electrodeposition of Ni was observed. It was found that $MgSO_4$ additives (Fig. 1.) increase the quantity of deposited Ni to a similar extent for both standard and acidified electrodeposition baths, with the increase being linear to the concentration of $MgSO_4$ used.

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EVALUATION OF PHYTOCHEMICALS AND ANTIOXIDANT ACTIVITY IN *CATHARANTHUS ROSEUS* CALLUS CULTURES

Ilona Jonuškienė[1,2]*, Monika Mazurkevičiūtė[1], Rima Stankevičienė[1], Neringa Petrašauskienė[3], Ingrida Tumosienė[1], Kristina Kantminienė[3]

[1] Department of Organic Chemistry, Kaunas University of Technology, Kaunas, Lithuania;
[2] Bioprocess Research Centre, Kaunas University of Technology, Kaunas, Lithuania;
[3] Department of Physical and Inorganic Chemistry, Kaunas University of Technology, Kaunas, Lithuania;
* *ilona.jonuskiene@ktu.lt*

Catharanthus roseus is a medicinal plant widely recognized for its important pharmacological properties and indole alkaloids [1]. It is a primary source of vinblastine and vincristine, which are used in chemotherapy to treat cancers such as breast and uterine cancers, as well as lymphomas. The plant has been used to treat conditions such as diabetes, hypertension, malaria, and skin conditions such as eczema and psoriasis. *Catharanthus roseus* extracts have shown promise as antimicrobial agents, particularly against antibiotic-resistant pathogens. The plant is rich in terpenoid indole alkaloids, including ajmalicine and serpentine, which are used to treat hypertension and other conditions. It also contains flavonoids, tannins, saponins, and steroids, all of which contribute to its pharmaceutical value [2–3]. Nowadays, techniques based on plant biotechnology provide a means of producing bioactive compounds from plants. These techniques allow for the direct production of these compounds through the aseptic growth of plant cells, tissues or organs, enabling the production of the desired bioproduct. *Catharanthus roseus* is a rich source of diverse phytochemicals with significant therapeutic potential, particularly for antioxidant and antimicrobial therapies [4].

One of the biotechnological objectives considered for *in vitro Catharanthus roseus* callus cultures was the production of phytochemical compounds. This study focused on the biological activity of these callus cultures. Callus cultures from leaves, stems and roots of *C. roseus* were cultivated in an MS medium supplemented with following plant growth hormones: 1-naphthaleneacetic acid (NAA), 6-furfurylaminopurine (kinetin), melatonin and the amino acid *L*-tryptophan. The highest concentrations of total phenolic compounds, flavonoids, and carotenoids were found in the leaf callus cultures grown in an MS medium containing NAA (1 mg/L), kinetin (0.1 mg/L) and *L*-tryptophan (0.5 mg/L). Extracts from stem callus cultures grown in an MS medium containing the phytohormones NAA (1 mg/L) and kinetin (0.1 mg/L) and *L*-tryptophan (0.5 mg/L), exhibited the highest antioxidant activity, as determined by the DPPH and FRAP methods.

Catharanthus roseus is a vital medicinal plant with significant biological activity and biotechnological potential. The green synthesis of nanoparticles using *Catharanthus roseus* extracts and research into nanotechnology-based drug delivery systems is also an emerging area [5].

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THERMAL PROCESSING OF CORN STARCH ESTERS USING NON-TOXIC PLASTICIZERS

Deimante Rosliuk[1]*, Dovilė Liudvinavičiūtė[1], Ayodeji Amobonye[1], Remo Merijs Meri[2], Laura Pečiulytė[1], Joana Bendoraitienė[1], Ramunė Rutkaitė[1], Shu-Kai Yeh[3]

[1] Department of Polymer Chemistry and Technology, Kaunas University of Technology, Lithuania
[2] Institute of Chemistry and Chemical Technology, Riga Technical University, Latvia
[3] Department of Materials Science and Engineering, National Taiwan University of Science and Technology, Taiwan
** deimante.rosliuk@ktu.lt*

The chemical modification of starch has become an effective way to adjust its physicochemical and thermal processing properties. Among the most widely used approaches, esterification using octenyl succinic anhydride (OSA) and acetic anhydride (AA) alters the molecular structure of starch. Such modification imparts amphiphilic character, reduces intermolecular hydrogen bonding, increases chain mobility. These structural changes help overcome the poor melt flow and brittleness of native starch, thereby improving its suitability for thermoplastic processing. Moreover, the addition of environmentally benign plasticizers enhances molecular mobility, thereby improving material flexibility. Overall, combining chemical modification with non-toxic plasticizers offers a promising strategy to optimize sustainable starch-based materials for thermal processing.

In this work, corn starch was esterified with OSA and AA, resulting in degrees of substitution of 0.026 and 2.02, respectively. The thermal extrusion of synthesized starch was studied at different processing temperatures (140, 160, and 180 °C) and by varying the type of plasticizer (triacetin, polyethylene glycol, or triethyl citrate) and its concentration (25–35 wt.%). The extrusion process efficiency was assessed by analysing specific mechanical energy (SME) values, while the melt flow and mechanical characteristics of the obtained materials were evaluated through standardized testing.

The temperature and the amount of plasticizer had only a minor impact on SME values, whereas the type of plasticizer significantly affected SME parameter. Melt flow index was highly dependent on both the type and concentration of the plasticizer, while extrusion temperature did not exhibit a significant effect. Finally, the mechanical properties were highly affected by plasticizer type, its concentration, and the processing temperature.

Acknowledgements. This work was supported by the Project of Scientific Cooperation Program between Latvia, Lithuania, and Taiwan "Biopolymer based green thermoplastic foams with improved biodegradability for sustainable material technologies (GREENPLAST)" and received funding from the Research Council of Lithuania (LMTLT), agreement No S-LLT-25-4, the Latvian Council of Science, agreement No LV-LTTW/2025/2, the National Science and Technology Council (NSTC), Republic of China (Taiwan), agreement No 114-2923-E-011-002-MY3.

INVESTIGATION OF PHOTOPHISICAL AND ELECTROLUMINESCENT PROPERTIES OF DONOR-ACCEPTOR LIGHT-EMITTING SEMICONDUCTORS EXHIBITING MECHANOLUMINESCENCE AND THERMALLY ACTIVATED DELAYED FLUORESCENCE

Lesia Volyniuk[1]*, Audrius Bucinskas[1], Stepan Kutsiy[2], Dmytro Volyniuk[1], Juozas V. Grazulevicius[1]

[1] Department of Polymer Chemistry and Technology, Kaunas University of Technology, Kaunas, Lithuania
[2] Department of Electronic Engineering, Lviv Polytechnic National University, Lviv, Ukraine
* *lesia.volyniuk@ktu.lt*

Donor-acceptor type light-emitting semiconductors can exhibit thermally activated delayed fluorescence (TADF), thereby facilitating the harvesting of triplet excitons under electrical excitation [1]. This property is useful for achieving 100% internal quantum efficiency in organic light-emitting diodes (OLEDs) [2]. However, the TADF efficiency of organic emitters is highly sensitive not only to chemical modifications of their molecular structures but also to external physical stimuli [3].

In this study, we aimed to investigate the effects of chemical modifications and physical stimuli on their photophysical and electroluminescent properties for four newly synthesized donor-acceptor compounds. The same acceptor, based on trifluoromethyl and benzonitrile units, and different donors containing phenothiazine or acridan. Powders of the compounds emit various colours of mechanoluminescence, ranging from bluish green to orange, depending on different molecular modifications and physical stimuli. The synthesized compounds demonstrate aggregation–induced emission enhancement, as evidenced by their higher photoluminescence quantum yields (PLQYs) in film form compared to solutions. TADF properties of the phenothiazine or acridan derivatives were investigated by steady-state and time-resolved spectroscopy at various temperatures. Compounds demonstrated bipolar charge transport, able to transport both holes and electrons with the higher mobilities of $3 \cdot 10^{-4}$ cm^2/Vs at the electric field of $6.4 \cdot 10^5$ V/cm. According to the photoelectron emission spectroscopy, the ionisation energies of the compounds are in the range between 5.67 eV and 6.14 eV. In the air, one compound showed a PLQY exceeding 50%. As a result, this compound showed a higher external quantum efficiency of 14.81 % when used as the emitter in simply structured OLEDs. Various effects of chemical modifications and physical stimuli on photophysical and electroluminescent properties for newly synthesized donor-acceptor compounds will be discussed at the conference. In more detail.

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EFFECT OF REACTION TIME ON THE FORMATION OF BEE POLLEN-MODIFIED HYDROXYAPATITE

Maab Elsheikh*, Inga Grigoraviciute, Zivile Stankeviciute, Aivaras Kareiva

Faculty of Chemistry and Geosciences, Institute of Chemistry, Vilnius, Lithuania
* *maab.ahmed@chgf.vu.lt*

Calcium hydroxyapatite (CHA; $Ca_{10}(PO_4)_6OH_2$) has been extensively studied due to its physicochemical versatility [1]. Nonetheless, the regulation of its surface properties remains a significant challenge, as these properties are influenced by the synthesis conditions, particularly in the presence of bio-derived additives [2]. In this study, bee pollen (BP), a natural source of biomolecules rich in polyphenols [3] was incorporated during the synthesis of CHA using a co-precipitation method to examine the effect of reaction time (4–120h) on the interaction between ion chemistry and structural development. X-ray diffraction (XRD) confirmed the formation of the apatite phase in all samples, with a reduction in peak intensities at intermediate reaction times >24 hours, indicating decreased crystallinity. Fourier-transform infrared (FTIR) spectroscopy revealed the presence of BP-derived functional groups without any significant alteration of the phosphate groups. Inductively coupled plasma optical emission spectroscopy (ICP/OES) demonstrated a reduction in the Ca/P ratio during the initial reaction phases, indicating Ca^{2+} chelation by BP and the formation of a calcium-deficient hydroxyapatite (CDHA; $Ca_9(HPO_4)$ $(PO_4)_5(OH)$), with partial recovery observed at extended reaction times. Brunauer-Emmett-Teller (BET) analysis revealed a nonlinear progression of surface properties due to the competing influences of pore blocking and particle size distribution. Meanwhile, thermogravimetric (TG) analysis verified the variability in organic content, reaching a peak at an intermediate reaction time, specifically at 24 hours.

These findings indicate that the reaction time is a key parameter for tuning the structural and surface properties of bee pollen–hydroxyapatite systems. Furthermore, the incorporation of BP makes these materials promising candidates for biomedical applications, such as bone tissue engineering and antibacterial coatings.

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TUNING INTERSYSTEM CROSSING IN TADF OLEDS VIA HALOGEN SUBSTITUTION OF MCP HOST MATERIALS

Karolis Leitonas*, Simas Mačionis, Jūratė Simokaitienė, Juozas Vidas Gražulevičius

Department of Polymer Chemistry and Technology, Kaunas University of Technology, Lithuania
** karolis.leitonas@ktu.lt*

The heavy atom effect in organic host materials represents an emerging strategy for enhancing the performance of thermally activated delayed fluorescence (TADF) organic light-emitting diodes (OLEDs). Halogen functionalization of host molecules can promote spin-orbit coupling (SOC), thereby accelerating intersystem crossing (ISC) and reverse intersystem crossing (RISC) processes critical for efficient triplet exciton harvesting [1,2]. While internal heavy atom effects in emitter molecules have been extensively studied, the systematic incorporation of halogens into host scaffolds and their external influence on TADF dopants remains insufficiently understood [3]. In this work, we investigate derivatives of the widely used OLED host material

1,3-bis(N-carbazolyl)benzene (mCP) – a well-established bipolar host with favorable triplet energy substituted with bromine (Br) or chlorine (Cl) atoms at selected positions on central phenyl ring. The study aims to elucidate how the type and position of halogen substituents influence the photophysical and electronic properties of these hosts. Steady-state and time-resolved photoluminescence spectroscopy, along with cryogenic measurements, will be employed to determine singlet and triplet energies and to extract radiative, non-radiative, and ISC rate constants. Selected TADF emitters will be doped into the halogenated mCP hosts to evaluate the external heavy atom effect on RISC rates and delayed fluorescence characteristics. OLED devices incorporating these host-dopant systems will be fabricated and characterized to assess the impact of halogenation on external quantum efficiency, turn-on voltage, and electroluminescence properties. This comprehensive optical-to-device investigation aims to establish structure-property relationships guiding the rational design of halogenated organic hosts for high-performance TADF OLEDs.

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SYNTHESIS OF PYRAZOLE AND BENZIMIDAZOLE DERIVATIVES ANNULATED THROUGH OXAZACYCLES

Agnė Užupytė*, Povilas Viltrakis, Vilija Kederienė, Algirdas Šačkus, Eglė Arbačiauskienė

Faculty of Chemical Technology, Kaunas University of Technology, Kaunas, Lithuania
* agne.uzupyte@ktu.edu

Heterocyclic compounds are fundamental to drug discovery because their adaptable structures offer wide-ranging possibilities for medicinal use [1,2]. Although pyrazole- or benzimidazole-fused heterocycles [3–5] and a range of six-, seven-, or eight-membered oxazacycles [6,7] have each been described separately, no polycyclic structures that integrate pyrazole, benzimidazole, and a tunable oxazacycle have been synthesized to date. The establishment of strategies to obtain these new fused frameworks offers a means to broaden the chemical space of biologically important heterocycles.

The main objective of this work is to establish a versatile and efficient synthetic approach to accessing new polycyclic structures that integrate pyrazole, benzimidazole, and various six-, seven-, or eight-membered oxazacycles. By doing so, this study aims to broaden the chemical space of biologically relevant heterocycles and generate new scaffolds for future possible pharmacological investigation.

Pyrazole–benzimidazole frameworks fused through various oxazacyclic systems were prepared using a two-step modular strategy. Initially, a pyrazole carbaldehyde was reacted with a diamine to generate a pyrazole–benzimidazole intermediate. In the second step, an annulation triggered by a dihalogenated alkane was employed to connect the pyrazole hydroxyl group to the benzimidazole NH group, thereby constructing the tetracyclic scaffold. Reactions were tracked by TLC and the identities of intermediates as well as final products were verified using NMR spectroscopy, mass spectrometry, and IR measurements. The modular two-step synthetic route efficiently produced a series of pyrazole–benzimidazole derivatives fused through oxazine, oxazepine, and oxazocine rings.

These findings highlight both the practicality and flexibility of the synthetic approach in generating previously unknown polycyclic scaffolds. This strategy broadens the chemical landscape of biologically significant heterocycles and establishes a basis for future investigations of their pharmacological properties.

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COPPER TIN SULFIDE FILMS: INFLUENCE OF SYNTHESIS METHOD ON STRUCTURAL AND MORPHOLOGICAL PROPERTIES

Dominyka Zubrickaitė, Asta Bronušienė, Ingrida Ancutienė*

Kaunas University of Technology, Kaunas, Lithuania
** ingrida.ancutiene@ktu.lt*

Currently, there is a search for semiconductor materials that are low-cost, abundant, non-toxic, and possess good optical efficiency. Ternary copper tin sulfides exhibit optimal optical properties, making them suitable for applications in photovoltaics, photocatalysis, and photodetectors [1–5]. The aim of this work was to synthesize copper tin sulfide films on glass substrates coated with fluorine-doped tin oxide (FTO) and to investigate the deposited and annealed films. The synthesis consisted of two stages: first, tin sulfide films were synthesized using a simple and easily performed successive ionic layer adsorption and reaction (SILAR) method. Then the deposited films were modified with copper(II) or copper(II/I) ions solutions. After deposition, the films were annealed at 200 ^{o}C, and the effect of annealing was observed.

To determine the phase composition of the deposited films, X-ray diffraction analysis of as-deposited and annealed samples was performed. The study examined the effect of varying numbers of cycles (20, 30 and 40) on the composition of tin sulfide films deposited on FTO glass, the effect of treatment in copper(II) or copper(II/I) ion solutions on the composition of the obtained films, and the effect of annealing in inert atmosphere on the composition of both tin sulfide and mixed copper-tin sulfide films. In this study, by varying the deposition conditions, copper tin sulfide films were synthesized, and the presence of tin(II) sulfide (SnS), mixed tin sulfide (Sn_2S_3), djurleite ($Cu_{31}S_{16}$), anilite (Cu_7S_4), and a mixed copper tin sulfide phase (Cu_4SnS_4) was detected. Additionally, a tin(IV) oxide phase was identified due to the thinness of the deposited films. It is important to note that annealing at low temperatures increased the crystallinity of the samples, although the phase composition remained unchanged. As the number of SILAR cycles increased, the surface morphology became more uniform, and longer treatment with copper ions reduced porosity and resulted in more homogeneous films with better particle size distribution. After annealing, the particles formed agglomerates, but the overall film remained more uniform. It was found that copper tin sulfides predominated in the formed films, although adsorbed atmospheric oxygen was also present, as confirmed by energy-dispersive spectroscopy. The study determined that after annealing, the electrical resistance increased from 45.3 Ω to 96.0 Ω, indicating that the non-annealed samples exhibited higher electrical conductivity.

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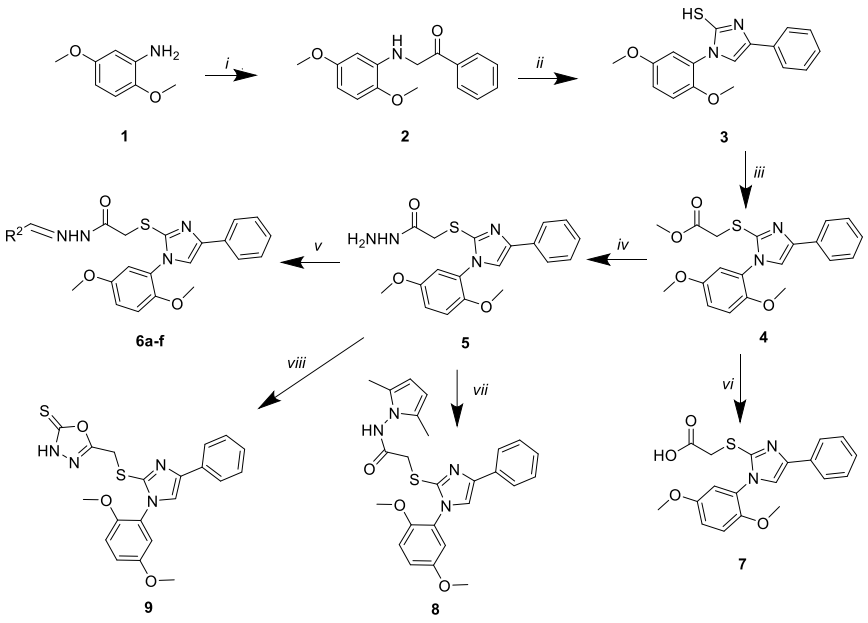
SYNTHESIS OF NOVEL 1,4-DISUBSTITUTED IMIDAZOL-2-THIOL DERIVATIVES

Birutė Sapijanskaitė-Banevič*, Tomas Tutkus

Department of Organic Chemistry, Kaunas University of Technology, Kaunas, Lithuania
** birute.sapijanskaite@ktu.lt*

Azoles are heterocyclic compounds with rising potential in medicinal chemistry. Among them, imidazole derivatives display a broad spectrum of biological activities, including antimicrobial, anticancer, antifungal, and anti-inflammatory effects [1].

In this work, precursor 3 was synthesized by reacting primary amine 1 with 2-bromoacetophenone in the presence of sodium bicarbonate, then the resulting aminoketone 2 was subsequently cyclized with KSCN under acidic conditions. To synthesize compound 4, imidazole-2-thiol 3 was treated with methyl bromoacetate in basic medium. Alkaline hydrolysis of methyl ester 4 yielded carboxylic acid derivative 7. Hydrazide 5 was prepared by reacting methyl ester 4 with hydrazine monohydrate in propan-2-ol.



Reagents and reaction conditions: *(i)* 2-bromoacetophenone, $NaHCO_3$, MeOH, 25 °C , 4 h; *(ii)* KSCN, $AcOH_{conc}$, Δ, 1 h; *(iii)* methyl bromoacetate, K_2CO_3, CH_3COONa, 1,4-dioxane, Δ, 1 h; *(iv)* $NH_2NH_2{\cdot}H_2O$, *i*-PrOH, Δ, 4 h; *(v)* corresponding aromatic aldehyde, $AcOH_{conc}$, *i*-PrOH, Δ, 2-5 h; *(vi)* $NaOH_{aq}$, Δ, 1 h; *(vii)* hexane-2,5-dione, $AcOH_{conc}$, *i*-PrOH, Δ, 4 h; *(viii)* 1. CS_2, KOH, MeOH, Δ, 5 h; 2. HCl_{aq} to pH 1.

Fig. 1. Synthesis of 1,4-disubstituted imdazol-2-thiol derivatives

Condensation of hydrazide 5 with various aromatic aldehydes produced hydrazones 6a-f, and with hexane-2,5-dione in the presence of an acid catalyst – pyrrole derivative 8. The intramolecular cyclization of acid hydrazide 5 with carbon disulfide was carried out and resulted in oxadiazole in 9 in 76%.

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EFFECT OF SiO_2 ADDITIVE AND HYDROTHERMAL SYNTHESIS CONDITIONS ON TRICALCIUM ALUMINATE HYDRATE FORMATION

Jolanta Doneliene*, Bartas Gedminas, Andzelika Aleinikovaite, Kristina Vasiliauskiene, Anatolijus Eisinas

Department of Silicate Technology. Kaunas University of Technology, Kaunas, Lithuania
** jolanta.doneliene@ktu.lt*

A main stable phase in a $CaO–Al_2O_3–H_2O$ system is tricalcium aluminate hydrate – katoite ($3CaO·Al_2O_3·6H_2O$ or C_3AH_6) [1]. It can be formed from refractory waste and calcium aluminate cement materials at the end of their life cycle [2]. Katoite can also be synthesised by mechanochemical processes [1] or by hydrothermal synthesis [3, 4]. Previous results [4] have shown that in an unstirred $CaO–Al_2O_3–H_2O$ suspension with molar ratio CaO/Al_2O_3=2.8, after hydrothermal synthesis at 130°C for 4 h, katoite was obtained and it fully recrystallised into mayenite at 350 °C. There is a lack of data on how the SiO_2 additive affects the formation and properties of tricalcium aluminate hydrate. This is especially relevant when using natural starting materials – CaO and Al_2O_3 – which are usually contaminated with SiO_2 impurities.
The aim of this work was to determine the SiO_2 additive influence on the formation of katoite and its thermal stability. The synthesis products were obtained using hydrothermal synthesis at 130°C for 1 h and unstirred suspensions with molar ratios of $CaO/(Al_2O_3+SiO_2)$=2.8 and SiO_2=0 or 0.25 (the liquid-to-solid ratios of all suspensions were 10:1). Thermal stability of the synthetic products was investigated using additional calcination at 350°C for 1 h with a high-temperature camera Nabertherm Model L5/11 (Nabertherm GmbH, Germany).

The results confirmed that the main synthesis product of the hydrothermal synthesis at 130°C for 1 h in the sample without SiO_2 was katoite. When the amount of SiO_2 additive increased, the main peak of katoite intercalated with SiO_2 increased. After additional calcination of the synthesis products, pure mayenite and mayenite intercalated with SiO_2 were formed. It was determined that the SiO_2 additive did not influence the thermal stability of the products: in both systems, synthetic katoite fully decomposed to mayenite at 350 °C. Prolonging the isothermal curing duration yielded similar results: after 72 h of synthesis, slight differences in diffraction peak intensities were observed. These results were also confirmed by the Proton Nuclear Magnetic Resonance (^{1}H NMR) spectroscopy. It can be assumed that SiO_2 additives were incorporated in the synthesis products' structure, because the diffraction peaks characteristic of tricalcium aluminum silicate hydrates or other types of hydrogarnets were not identified in the XRD curves.

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THE INFLUENCE OF RAW AND WATER – WASHED BYPASS DUST ON THE PROPERTIES OF CONCRETE HARDENING IN CO_2 ENVIRONMENT

Neda Aliukonytė*, Raimundas Šiaučiūnas

Department of Silicate Technology, Kaunas University of Technology, Kaunas, Lithuania
* *neda.aliukonyte@ktu.edu*

Concrete is the second most widely used product in the world after water. Due to the high and growing demand for construction materials, the cement industry is responsible for approximately 5–7% of all human-caused greenhouse gas emissions worldwide [1]. The search for new alternative cementitious materials with a lower carbon footprint than ordinary Portland cement (OPC) is one of the biggest challenges facing the cement industry.

Raw materials used: CEM 1 42.5 R, CEN standard sand EN 196-1 and SC Akmenės cementas Bypass dust. A part of the Bypass dust was washed with water because it contains potassium chloride, which has a negative impact on the performance characteristics of concrete. Raw additive was washed using a solid : water ratio of 1:10 (by mass) for 10 minutes at 40 °C. XRD analysis shows that the Bypass dust contains sylvite (KCl), spurite, calcite, portlandite, alite, and larnite. The water-washed dust no longer contains sylvite. The samples were compressed with a force of 12.5 kN from OPC : sand (1:3 by mass) mixtures, in which 0; 5; 10; 15 and 20% OPC replaced with raw or washed Bypass dust. They were cured in a reactor filled with 99.9% pure CO_2 gas at temperature of 25, 35, 40 and 45°C, under a pressure of 12.5 bar. Holding time was 24 h. It is recommended to cure the samples at 45 °C, as this temperature resulted in the highest strength values. The data on their properties are presented in Table 1.

Table 1. Dependence of sample properties on the amount of raw and water-washed Bypass dust

Amount of bypass dust, %	Compressive strength, MPa	Amount of bound CO_2, %	Compressive strength, MPa	Amount of bound CO_2, %
	Raw Bypass dust		Water-washed Bypass dust	
0	32.50	6.03	32.50	6.11
5	-	-	32.29	6.46
10	31.14	5.87	32.86	6.47
15	-	-	25.71	6.43
20	21.95	4.99	27.49	6.75

XRD analysis of carbonated samples revealed that in the mixtures containing raw dust, sylvite and quartz remains, calcite forms and the intensity of the alite peaks decreases. Whereas in the samples containing washed dust, silvite was no longer present and tricalcium pentaoxysilicate was additionally formed.

The results showed that samples with washed dust had higher compressive strength than those with raw dust and did not contain soluble compounds that could harm concrete quality. These mixtures are suitable for C25/30 (medium - strength) concrete and can help significantly reduce CO_2 emissions.

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SYNTHESIS OF 1.13 nm TOBERMORITE AND XONOTLITE FROM MICROSILICA

Liveta Steponaitytė*, Raimundas Šiaučiūnas

Department of Silicate Technology, Kaunas University of Technology, Kaunas, Lithuania
** liveta.steponaityte@ktu.lt*

Microsilica is an amorphous material formed during the production of silicon or iron-silicon alloys by reducing quartz with carbon-containing materials such as coal, coke, wood chips, and others. Microsilica is characterized by its insulating qualities and has stable physical and chemical properties. [1]. The reactivity of the raw materials affects the rate of interaction between SiO_2 and CaO. Amorphous silicon dioxide dissolves faster than crystalline SiO_2, thereby accelerating the formation of low-base calcium silicate hydrates (C-S-H) [2]. The main C-S-H phases, xonotlite and 1.13 nm tobermorite, formed in dense silicate and insulating autoclaved products. These compounds show thermal stability and enhance mechanical strength, durability, and structural stability. The main difference is that tobermorite-dominated materials are thermally stable up to 700 °C while xonotlite-dominated products are stable up to 1100 °C [3]. Microsilica is a raw material for synthesizing compounds suitable to produce heat-resistant insulating materials.

Source of SiO_2 used in the work: microsilica (Mikrosill Gray, RUFAX, Lithuania). The X-ray analysis shows no diffraction peaks, only a saddle, which indicates that microsilica is an amorphous material. Microsilica was milled in a vibrating planetary mill Fritsch Pulverisette 9 (Fritsch GmbH, Germany) for 2 min at 900 rpm. The specific surface area (S_a) is 3514,17 $m^2 \cdot kg^{-1}$. CaO was obtained by burning the reagent $CaCO_3$ for 1 h at 950 °C (CaO_{free} = ~99%). Hydrothermal syntheses were carried out in stirred suspensions (100 rpm) in autoclave (Parr Instruments, model 4751, USA) at 180 °C for 2–48 h (the water/solid ratio was equal to 20). The mixtures with molar ratio CaO/SiO_2 = 0.83 were prepared in a homogenizer Turbula Type T2F (Willy A Bachofen AG, Switzerland) for 45 min at 49 rpm.

After 2 h of hydrothermal synthesis, portlandite traces are detected and C-S-H (I) is formed. When the synthesis was extended to 4 h, no significant changes were observed, except that all portlandite reacted. The 1.13 nm tobermorite peaks and traces of xonotlite were observed after 8 h of hydrothermal synthesis. When the synthesis duration was prolonged to 16 h, the amount of these C-S-H enhanced as the intensity of their peaks in the XRD pattern increased significantly. By extending the synthesis time to 48 h, more of the thermodynamically most stable C-S-H (xonotlite) is formed while the intensity of the 1.13 nm tobermorite peaks decreases.

Therefore, microsilica is much more reactive under hydrothermal conditions than the reagent $SiO_2 \cdot nH_2O$, with which we were unable to obtain xonotlite under identical synthesis conditions [4]. In conclusion, microsilica is perfectly suited for the synthesis of calcium silicate hydrates, from which heat-resistant insulating materials are produced.

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THERMAL-INDUCED PERFORMANCE ENHANCEMENT IN SPRAY-PYROLYZED Sb2S3 PHOTOVOLTAICS

Ernest A. Asare[1]*, Robert Aleksander Liiv[1], Atanas Katerski[1], Christopher Don[1], Raavo Josepson[1], Alex Jimenez Arguijo[2], Edgardo Saucedo[2], Nicolae Spalatu[1], Malle Krunks[1], Ilona Oja Acik

[1] Tallinn University of Technology Tallinn, Estonia
[2] Polytechnic University of Catalonia (UPC), Barcelona, Spain
* *ernest.asare@taltech.ee*

As research into sustainable photovoltaics accelerates, environmentally friendly antimony trisulfide (Sb_2S_3) thin-film has emerged as high-potential material due to their optimal bandgap of 1.7 eV and earth-abundant composition. However, their efficiency is limited by a persistent open-circuit voltage (V_{OC}) deficit, which is primarily driven by non-radiative recombination at bulk defects and the absorber/transport layer interfaces. Fabrication methods such as chemical bath deposition (CBD), hydrothermal synthesis, and ultrasonic spray pyrolysis (USP) often yield amorphous or low-crystalline quality films that require a post-annealing step to achieve the optimal orthorhombic crystalline phase and morphology for photovoltaic applications. While annealing temperature is well-explored, the role of annealing duration (or time) in mitigating these defects remains under-explored.

In this work, we address this gap by presenting a systematic investigation into the effect of annealing time on the performance and defect physics of Sb_2S_3 solar cells fabricated via USP deposition technique. By maintaining a constant substrate annealing temperature of 300 °C and varying durations from 6 to 18 minutes, we identify a performance peak at 12 minutes. This optimized device achieving a power conversion efficiency (PCE) of 6.12 % with a short-circuit current density (J_{SC}) of 14.8 $mAcm^{-2}$, a fill factor of 60% and a V_{OC} of 718 mV. Remarkably, the 18 minute duration yielded a peak V_{OC} of 734 mV, representing one of the highest reported values for USP-deposited Sb_2S_3, although a trade-off in current density was observed due to sublimative thining of the absorber.

Advanced characterization, including temperature-dependent current density-voltage (J-V-T) measurements, Suns-Voc, impedance spectroscopy, and capacitance-voltage (C-V) analysis, reveals that extended annealing promotes significant interface passivation. This kinetic control facilitates interfacial optimization and the formation of a stable, self-passivated interface that suppresses trap-assisted recombination which directly accounts for the observed increase in V_{OC} and overall device performance. Our findings emphasize the critical role of kinetic control in thermal processing for overcoming the Voc deficit in emerging thin-films photovoltaics.

HORIZONTALLY ORIENTED PYRIDO[2,3-B]PYRAZINE EMITTERS FOR EFFICIENT OLEDS

Matas Gužauskas*, Domantas Lekavičius, Rasa Keruckienė, Dmytro Volyniuk, Juozas V. Gražulevičius

Department of Polymer Chemistry and Technology, Kaunas University of Technology, Lithuania
** matas.guzauskas@ktu.lt*

The search for organic semiconductors with an ideal combination of charge-transporting, exciton-harvesting, and light-emitting properties is vital for efficient organic light-emitting diodes (OLEDs) [1]. This study examines the light-emitting properties and potential applications of new pyrido[2,3-b]pyrazine derivatives. Four donor-acceptor emitters containing carbazole or phenothiazine donor groups were synthesized. A full study of their photophysical behavior revealed that these compounds emit conformer-assisted blue-to-red light. They demonstrate strong thermally activated delayed fluorescence (TADF) properties, supported by small energy differences between singlet and triplet states (ΔE_{ST}) dropping as low as 0.16 eV. This facilitates efficient reverse intersystem crossing, allowing photoluminescence quantum yields to reach up to 82%.

A major advantage of these new emitters is their tendency to adopt horizontal molecular orientation in thin films, with horizontal orientation order parameters (Θ_H) reaching up to 0.90. This alignment improves the internal light outcoupling efficiency of the devices [2]. Additionally, the compounds show valuable bipolar charge transport capabilities, exhibiting hole mobilities up to 3.8×10-4 $cm^2/V{\cdot}s$ and electron mobilities up to 4.6×10-5 $cm^2/V{\cdot}s$.

The application of these new pyrido[2,3-b]pyrazine-based emitters inside actual OLED devices was highly successful. When optimized using a host-guest system, the resulting devices exhibited a high internal quantum efficiency of up to 82% and reached a maximum external quantum efficiency (EQE) of 21.3%, alongside a current efficiency of 52.5 cd/A. These findings indicate that this molecular design strategy produces highly efficient, horizontally oriented emitters suitable for modern optoelectronic applications.

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EFFICIENT MICROWAVE-ASSISTED SYNTHESIS AND CHARACTERIZATION OF C- and O-DOPED BORON NITRIDE QUANTUM DOTS

Giedrė Grincienė*, Renata Karpicz, Katsiaryna Chernyakova, Ieva Matulaitienė, Raimondas Giraitis

Center for Physical Sciences and Technology, Vilnius, Lithuania
* *giedre.grinciene@ftmc.lt*

In recent years, Boron Nitride Quantum Dots (BNQDs) have emerged as a compelling alternative to traditional semiconductor quantum dots, which often contain toxic heavy metals. Due to their exceptional chemical stability, inherent biocompatibility, and robust photoluminescence, BNQDs are highly promising candidates for optical bio-imaging and cellular diagnostics. The relevance of this study is driven by the need to develop efficient, low-energy synthesis routes, such as microwave-assisted activation, that allow for precise control over the defect-mediated electronic structure and optical properties of BNQDs, optimizing them for practical biomedical applications [1–3].

In this work, a microwave-assisted solid-state synthesis was utilized to produce Boron Nitride (BN) nanostructures using boric acid and an excess of urea as precursors. To evaluate the phase evolution and structural transformation, the synthesis temperature was varied between 200 °C and 250 °C, with reaction durations ranging from 15 to 120 minutes. Subsequently, post-synthetic thermal annealing was performed in an inert Argon atmosphere at temperatures of 400 °C and 600 °C to stabilize the crystal lattice and optimize the luminescent properties.

Comprehensive spectroscopic analysis (FTIR and Raman) combined with emission spectra revealed that varying the synthesis conditions leads to the formation of BNQDs with diverse carbon-doping levels and defect densities. The results indicate that the synthesis temperature and reaction time directly influence the degree of carbon incorporation and surface functionalization, which in turn modulates the optical characteristics and colloidal stability of the quantum dots. These findings demonstrate that an optimized annealing regime is a critical factor in achieving stable photoluminescence, essential for their potential application as fluorescent biomarkers.

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PLASMA-ASSISTED ALGINATE COATINGS FOR POLYESTER SURFACE STABILISATION

Zeenat Fatima Iqbal*, Julija Baltušnikaitė-Guzaitienė

Department of Textile Technologies, State Research Institute Center for Physical Sciences and Technology, Kaunas, Lithuania
* *zeenat.iqbal@ftmc.lt*

Plasma treatment of textiles is a dry, environmentally friendly, and work-safe technique for surface modification that preserves the bulk properties of the material. This process modifies the fabric surface by introducing reactive functional groups, thereby enhancing its binding and adhesion characteristics. Improved adhesion may contribute to reduced fiber release, highlighting the importance of surface coating for fiber stabilization in synthetic textiles. In this study, knitted polyester fabric was subjected to plasma treatment to activate its surface and improve the adhesion of subsequent coatings. The plasma processing parameters were optimized at 100 W power, 40 Pa base pressure, and 120 s treatment time. In addition to the optimized conditions, alternative plasma parameter sets were also investigated to evaluate their influence on surface modification, specifically 120 W power with 90 s treatment time at 40 Pa and 120 W power with 75 s treatment time at an elevated base pressure of 60 Pa. On the other hand, a comparative study was also made to assess the alginate coatings on untreated plasma surfaces as well. Following plasma activation, the fabrics were coated with sodium alginate (Na-alginate) solutions at concentrations of 0.5%, 1%, and 1.5% using dip-padding to ensure uniform application as a biopolymer-based approach for surface encapsulation. Subsequently, the coated samples were crosslinked with a 0.1 M calcium chloride dihydrate solution to improve coating stability and impart hydrophobicity. Enhanced coating stability is particularly relevant for limiting fiber detachment under mechanical stress. The treated fabrics were then cured at 120 °C for 5 minutes to facilitate crosslinking and fixation of the coating onto the fiber surface.

The resulting modified fabrics were characterized using FTIR, SEM, and wettability measurements to evaluate chemical interactions, surface morphology, and changes in surface properties. Coating deposition was estimated from the weight difference before and after treatment, indicating coating coverage on the fiber surface. In conclusion, plasma treatment can be considered a promising and eco-friendly technique for surface modification, facilitating improved adhesion and performance of biopolymeric coatings, with potential relevance for reducing microplastic release from synthetic textiles through enhanced fiber surface stabilization.

ADVANCED LEATHER PROCESSING: SIMULTANEOUS SALT-FREE PICKLING AND BATING OF HIDE

Renata Biškauskaitė Ulinskė[1], Viktoriia Plavan[2], Virgilijus Valeika[1]*

[1] Kaunas University of Technology, Kaunas, Lithuania,
[2] Kyiv National University of Technologies and Design, Kyiv, Ukraine
* *virgilijus.valeika@ktu.lt*

The main aim of the study was to investigate a new salt-free hide pickling-bating by determining the influence of process parameters on changes in hide properties, as well as on chroming and wet-finishing processes.

The new method of hide pickling-bating using 2% *p*-toluenesulphonic acid monohydrate (*p*TsOH) and 0.05% Zime SB or 0.05% Oropon DVP enzyme preparations (EP) allowing an avoidance the use of sodium chloride and to reduce processing time by 1.75 hours was developed. A hide after experimental process has a 7.2-8.4 °C higher shrinkage temperature and the solutions contain 58-62% less dissolved particles and 92% less Cl^- comparing with the conventional process.

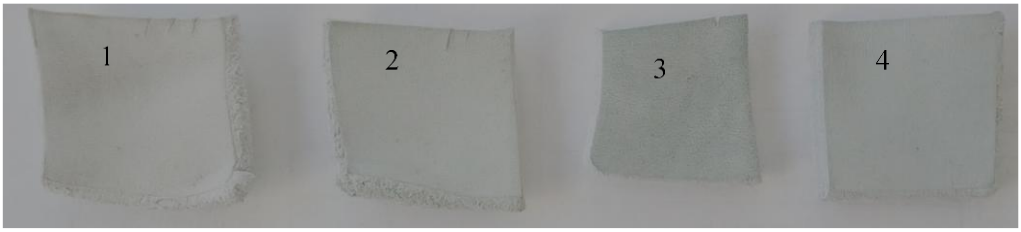

Fig 1. Chromed tanned leather (pickling method: 1 – control; 2 – *p*TsOH; 3 – *p*TsOH + EP Oropon DVP 0.05%; 4 – *p*TsOH + EP Zime SB 0.05%

Table 1. Dependence of chroming and chrome tanned leather properties on hide pickling method

Pickling method	Indexes			
	Shrinkage temperature, °C	Leather pH after chroming	Cr_2O_3 amount in leather, %	Cr_2O_3 exhaustion, %
*p*TsOH + EP Zime SB 0.05%	107.3±0.43	3.76±0.10	5.28±0.21	98.71±0.41
*p*TsOH + EP Oropon DVP 0.05%	102.0±0.50	3.73±0.15	5.46±0.20	99.88±0.77
*p*TsOH	108.0±0.50	3.09±0.10	4.73±0.16	98.37±0.85
Control	97.9±0.87	2.94±0.15	3.52±0.14	68.70±1.30

Chrome tanned semi-product (Fig. 1) after newly developed pickling results (Table 1) in higher tensile strength, higher shrinkage temperature and higher content of chromium compounds (5.3-5.5%) as well as better chromium exhaustion during chroming (up to 99.8%).

Wet-finishing processes did not show clear dependence of the dye consumption on the treatment method, but after pickling-bating, lower amount of fat liquoring materials was found in chrome tanned leather. This should be considered to improve the technology.

ADJUSTING THE MECHANICAL BEHAVIOR OF ACRYLIC-URETHANE POLYMER SYSTEMS

Artem Kolodiy[1], Viktoriia Plavan[1]*, Virgilijus Valeika[2], Iryna Liashok[1]

[1]Kyiv National University of Technologies and Design, Ukraine
[2]Kaunas University of Technology, Lithuania
* *plavan.vp@knutd.edu.ua*

Based on the results of the study of the physical and mechanical properties of acrylic-urethane polymer systems, it was concluded that increasing the polyurethane content up to 40% (by dry residue) in polymer systems is accompanied by an increase in the tensile strength of the films as well as their elongation at break. This improvement in the strength of acrylic-urethane systems may be attributed to the formation of additional intermolecular bonds, which leads to reduced mobility of molecular chains. The possibility of strong intermolecular interactions is confirmed by the increased resistance of acrylic-urethane compositions to ethanol. At a polyurethane content of 30–50% (by dry residue), swelling of acrylic-urethane films in ethanol is observed, while further increase in polyurethane content results in gradual dissolution of the films. This behaviour is likely due to the increased affinity of acrylic-urethane films for the polar solvent (ethanol) with higher polyurethane content, promoting a transition from limited swelling to complete dissolution as a result of the disruption of interchain interactions and a decrease in effective crosslink density.

Based on the analysis of the stress–strain curve (Fig. 1), which characterizes the behaviour of polymer materials under applied stress and deformation, it was concluded that the studied acrylic-urethane system exhibits pronounced viscoelastic properties. The curve demonstrates typical behaviour of polymers possessing both high strength and significant plasticity/elasticity. The combination of rigid acrylic segments and flexible urethane segments in acrylic-urethane systems provides a balance between stiffness and elasticity. The presence of 30–40% polyurethane (by dry residue) in the acrylic-polyurethane composition allows an increase in tensile strength up to 12.9–13.3 MPa, along with a simultaneous increase in elongation to 420–450%, compared to a film based on pure acrylic dispersion (tensile strength of 10.5 MPa and elongation of 233.3%).

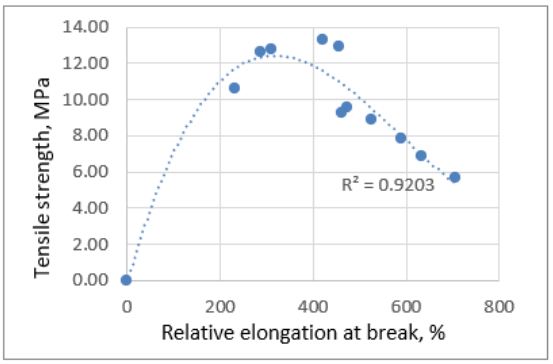

Fig. 1. Stress–strain curve for acrylic-urethane films

Thus, by varying the polyurethane content in acrylic-urethane polymer dispersions, it is possible to obtain textile coatings with the required physical and mechanical properties for specialized applications.

PRODUCTION OF GRANULAR BIO FERTILIZER

Kristina Jančaitienė*, Arminas Strolia

Department of Physical and Inorganic Chemistry, Kaunas University of Technology, Kaunas, Lithuania
* *kristina.jancaitiene@ktu.lt*

Organic granular fertilizer is an all-natural, environmentally friendly product designed to help plants grow healthier and stronger. This fertilizer contains a balanced blend of nitrogen, phosphorus and potassium (NPK) which promotes root development, improves water retention and increases plant vitality. In the production of NPK fertilizers, mineral raw materials are most often used, but alternatives are increasingly sought – such as by-products or ash from certain industries. Ash, which is formed by burning biomass or other organic waste, has a valuable nutritional composition - it contains calcium, potassium, phosphorus and trace elements. For this reason, ash can be used as a raw material in the production of fertilizers. However, it is necessary to assess the possible presence of pollutants, especially heavy metals – their concentrations are strictly regulated, therefore, a detailed chemical analysis must be performed before use [1].

In this study, the concentration of plant-available macronutrients (nitrogen, phosphorus and potassium) in various organic raw materials (banana peels and buckwheat hull ash) was determined and their use for the production of granular biofertilizers was evaluated. Granulation was carried out using a drum granulator-dryer and the properties of the granules were analyzed.

Granulation was also performed using only buckwheat hull ash to produce a granular fertilizer without additional organic additives. The data showed that pure ash formed brittle pellets that easily disintegrated, and particle adhesion was limited. Banana peels were used as an organic binder with a high sugar and polysaccharide content. Banana peel pulp acts as a strong but locally distributed organic binder. Due to the uneven distribution of sugars and polysaccharides in the mixture, two types of granules were formed:

- very strong granules formed locally in binder-rich zones;
- weak or non-formed granules in which the binder concentration was insufficient.

Experiments have shown that even a 5% banana peels addition significantly increases the average granule strength, but this is only due to 4–5 granules with higher strength, with values reaching 40 N/gran or even 70 N/gran, while most of the remaining results were recorded as 0 N/gran. Based on the obtained results, it can be concluded that the best outcome was achieved by combining buckwheat hull ash and banana peels in the granulation process.

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EFFECT OF COOKING ON *IN VITRO* PROTEIN DIGESTIBILITY OF MEAT IN ADULT AND ELDERLY GASTROINTESTINAL MODELS

Roberta Spangelytė, Ina Jasutienė*, Daiva Leskauskaitė

Kaunas University of Technology, Kaunas, Lithuania
* *ina.jasutiene@ktu.lt*

Proteins are essential dietary components involved in metabolism, tissue repair, and muscle maintenance [1–3]. While the recommended protein intake for adults is 0.8 g/kg/day, older adults are advised to consume 1.0–1.2 g/kg/day due to age-related declines in digestive efficiency and increased risk of sarcopenia. Chicken meat is a high-quality protein source with a favorable indispensable amino acid profile and high intrinsic digestibility. However, thermal processing may alter protein structure, enzyme accessibility, and amino acid bioavailability, thereby affecting digestibility [4,5].

This study evaluated the effects of thermal processing on the digestibility and amino acid bioaccessibility of chicken breast protein under simulated adult and elderly gastrointestinal conditions using the INFOGEST in vitro digestion model [6]. Protein digestibility was evaluated by soluble nitrogen, bioaccesible nitrogen, degree of hydrolysis, amino acid composition, free amino acid content and calculation of Predicted Protein Digestibility-Corrected Amino Acid Score (PDCAAS).

Crude protein content ranged from 19% to 24%, with the highest values in samples treated at 100 °C for 30 min. The degree of hydrolysis increased during digestion, with limited proteolysis during the gastric phase and markedly higher hydrolysis during the intestinal phase. The highest final hydrolysis values were observed in raw samples and those treated at 65 °C for 2 h. In the adult model, hydrolysis did not differ significantly among 65 °C treatments, whereas in the elderly model it increased with heating time. Overall digestibility ranged from approximately 52% to 91%, with the highest values in raw samples, followed by samples treated at 65 °C for 1 h. The bioaccessible peptide fraction (<10 kDa) ranged from 13% to 22% and followed similar trends. Raw chicken breast showed the highest amino acid release during digestion, followed by samples treated at 65 °C for 30 min, whereas treatment at 120 °C reduced amino acid release. Essential amino acid release was generally preserved after mild heating but was lower under elderly digestion conditions. These results indicate that protein digestibility and amino acid bioaccessibility of chicken breast are strongly influenced by both thermal processing and age-related digestive capacity.

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CO_2 CURING POTENTIAL IN HIDTRATED BLENDED CEMENT PRODUCTS

Žaneta Vadvilavičienė*, Raimundas Šiaučiūnas

Department of Silicate Technology, Kaunas University of Technology, Kaunas, Lithuania
* *zaneta.vadvilaviciene@ktu.edu*

The cement industry emits large amount of greenhouse gases (CO_2) [1, 2]. For this reason, the scientific and industrial communities colaborates to investigate how eficiantly reduce the amount of clinker in cement-based systems and to and find the best way to capture and utilize CO_2. The main issue of this work is to use externally collected CO_2 for the carbonation of blended cement samples. The raw materials used in this initial study are: clinker and gypsum (Slite Manufactor, Sweden) and sedimentary rock Opoka (Stoniškiai quary, Lithuania). The methods used in this work were: standard cement tests according EN standards (EN 196-3, EN 196-1), instrumental analysis (XRF, XRD, SEM, and calcimetry). Carbonation was performed after 48 h of curing under standard (hydraulic) curing conditions. Curing in CO_2 environment lasts for 24 h at 45 °C temperature and different pressures. Tests results shows that blended cement specimens can absorb approximately 4–7 % CO_2 during carbonization. Compressive strength of carbonated samples increases by up to 45 % compared to the non-carbonated 48 h (Table 1).

Table 1. Carbonation conditions and results. Blended cement composition 85% Clinker (in which 4% gypsium) +15% Opoka

Pressure, bar	Compressive strength, MPa			CO_2 absorption, %	Mass loss, %
	48 h EN 196-1 + 24 h, 45 °C, CO_2	Standard EN 196-1 hardening conditions			
		2 days	7 days		
5	44.8	25.4	41.6	4.3	1.10
12.5	43.1			6.7	0.25

These results indicates that carbonation after hidraulic curing can significantly accelerate the early compressive strength and reduces production time. After a three-day total curing period, the standard compressive strength of the blended cement specimens is achieved [3]. Our future research will focus on optimal conditions of hydratation and carbonation reactions. The final aim is applying this method in industrial scale.

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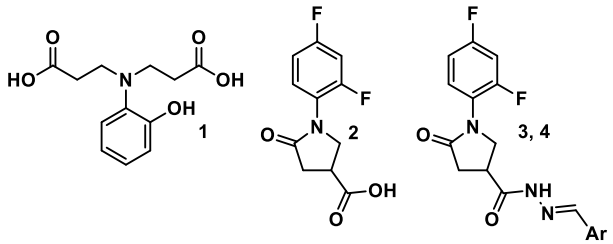
IDENTIFICATION OF SMALL-MOLECULE INHIBITORS TARGETING THE SOS RESPONSE IN *PSEUDOMONAS AERUGINOSA*

Guoda Pranaitytė[1], Birutė Grybaitė[1]*, Povilas Kavaliauskas[1], Waldo Acevedo[2], Ramunė Grigalevičiūtė[3], Vidmantas Petraitis[4], Rūta Petraitienė[4], Vytautas Mickevičius[1]

[1] Department of Organic Chemistry, Kaunas University of Technology, Radvilenų Rd. 19, Kaunas, Lithuania
[2] Institute of Chemistry, Faculty of Sciences, Pontificia Universidad Católica de Valparaíso, Chile
[3] Biological Research Center, Lithuanian University of Health Sciences, Kaunas, Lithuania
[4] Center for Discovery and Innovation, Hackensack Meridian Health, Nutley, USA
** birute.grybaite@ktu.lt*

The bacterial SOS response is a highly conserved DNA damage-induced regulatory pathway that promotes mutagenesis, genomic plasticity, and the emergence of antimicrobial resistance. In *Pseudomonas aeruginosa*, activation of the RecA–LexA axis contributes to antibiotic tolerance, highlighting this pathway as an attractive target for the development of resistance-modifying agents. In this study, a focused library of 517 drug-like small molecules was screened using a whole-cell *P. aeruginosa* reporter strain harboring a lexA-GFP construct under mitomycin C (MMC)-induced DNA damage. Compounds were prioritized based on selective inhibition of SOS activation while preserving bacterial viability. Four structurally diverse hits were identified, including a dipropionic acid (1), a pyrrolidinone carboxylic acid scaffold (2), and two hydrazone-linked pyrrolidinone derivatives (3 and 4), bearing electron-withdrawing fluoro and electron-donating dimethylamino substituents, respectively.



3 Ar = 4-F-C_6H_4; 4 Ar = 4-$(CH_3)_2$-C_6H_4;

Fig. 1. Structures of tested compounds (1–4)

Molecular docking studies revealed that the active compounds bind within a flexible regulatory loop of LexA, forming key hydrogen bond interactions with Arg105 and Arg204, alongside halogen bonding and hydrophobic contacts. Notably, the hydrazone derivatives 3 and 4 exhibited more favorable predicted binding energies, consistent with their extended conjugation and increased interaction potential within the binding pocket. Follow-up biological validation demonstrated that two lead compounds, particularly the hydrazone-based scaffolds, significantly (*p-value*<0.05) suppressed SOS induction in both PAO1 and PAK strains under MMC and ciprofloxacin treatment, indicating activity across multiple genotoxic stress conditions. All hit compounds demonstrated low cytotoxicity in A549, Vero, and HSAEC-1 cell lines. Taken together, these results highlight hydrazone-functionalized pyrrolidinone scaffolds as promising chemotypes for modulation of the *P. aeruginosa* SOS response and provide a foundation for the rational design of novel antibiotic adjuvants targeting adaptive resistance mechanisms in multidrug-resistant Gram-negative pathogens.

Acknowledgements. The research was funded by the Research Council of Lithuania (LMT) under project Nº S-MIP-25-21/ P-MIP-25-362.

SYNTHESIS OF NOVEL BENZOTHIAZOLE-BASED ARYLAMINE HOLE-TRANSPORTING MATERIALS FOR PEROVSKITE SOLAR CELLS

Povilas Luizys[1]*, Shun Tian[2], Kasparas Rakstys[1], Roland C. Turnell-Ritson[3], Valdas Paulauskas[4], Vygintas Jankauskas[5], Vytautas Getautis[1] and Mohammad Khaja Nazeeruddin[2]

[1] Kaunas University of Technology, Kaunas, Lithuania
[2] École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland
[3] Chemistry Research Laboratory, Oxford, United Kingdom
[4] Vytautas Magnus University, Kaunas, Lithuania
[5] Vilnius University, Vilnius, Lithuania
* *povilas.luizys@ktu.lt*

In recent decades, increasing energy demand has become a major global challenge. To meet these growing energy needs, various renewable energy sources have been explored. Among them, solar energy stands out for its potential to supply global energy demands. Currently, the most widely used solar cells are silicon-based, however, their production is energy-intensive and relatively complex.[1] Therefore, alternative photovoltaic technologies are being actively pursued. One of them is perovskite solar cells (PSCs), which have rapidly emerged as a key focus in photovoltaic research. Since their first demonstration in 2009 by Kojima and co-workers,[2] the performance of PSCs has improved significantly, reaching an efficiency of 27.3%.[3]

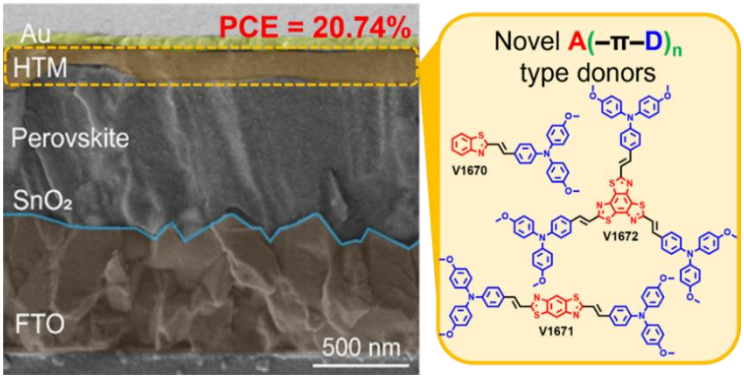


Fig. 1. The cross-sectional SEM image of the n-i-p structure PSC and chemical structure of target HTMs

The performance of PSCs is partially influenced by the properties of the hole transporting material (HTM) used. Here, we present the study of novel benzothiazole-based arylamines HTMs. The compounds are thermally stable (>350 °C) and exist in amorphous states. Their ionization potential fall within the range of 5.26–5.62 eV. PSCs employing the best performing HTM resulted in an efficiency of 20.74%. With this we report donor–π-bridge–acceptor type-strategy as an effective method to increase charge transport properties of HTMs, thereby improving performance of the hole transporting layer in PSCs.

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MORPHOLOGY AND CORROSIONS RESISTANCE OF PHOSPHATED MANGANESE ELECTRODEPOSITS OBTAINED FROM SULFATE BATH AT DIFFERENT TEMPERATURES

Vasaris Statkevičius, Egidijus Griškonis, Nerita Žmuidzinavičienė*

Department of Physical and Inorganic Chemistry, Kaunas University of Technology, Lithuania
** nerita.zmuidzinaviciene@ktu.lt*

Electrochemical deposition is a low-energy process, but it faces difficulties with manganese in particular due to manganese electronegativity (E^0 = -1.18 V vs. SHE). Additives such as group VI elements (Te, Se, S) are essential as they have shown to improve the efficiency of manganese electrochemical deposition [1]. Research on tellurium compounds is scarce and by researching it a middle ground between the other 2 additive benefits could be found. Manganese coatings show adequate corrosion resistance, but don't match its alloys properties [2]. Phosphating process [3] is used to enhance coatings corrosion resistance by converting surface into a rough amorphous or crystalline phosphate composite.

A substrate of carbon steel (ASTM A283) plates (8 cm^2) was used, electrochemical deposition was carried out in ammonium-manganese sulfate electrolyte (ASME) containing the mixture of $MnSO_4$ and $(NH_4)_2SO_4$ $5H_2O$. Sodium tellurate ($Na_2TeO_4 \cdot 2H_2O$) was used as electrolyte additive; pH was maintained around ~2.33. During electrochemical deposition two anodes, coated with lead(IV) oxide (Pb/PbO_2), and polyvinylchloride (PVC) woven membrane, separating the anode and cathode compartments, were used. Deposition lasted for 7 minutes with a cathodic current density of 15 A/dm^2, at temperatures of 20, 40, 60, 80 °C. Phosphating process was carried out at room temperature at around ~21 °C for 20 minutes. Phosphating solution consisted: $NaNO_3$, H_3PO_4, $Zn(NO_3)_2$; pH was maintained around ~2.35.

XRD analysis show that the coatings are predominantly composed of zinc phosphates and α-Mn. EDX analysis shows the discrepancies of elemental mass percentage of zinc, manganese, tellurium elements depending on analyzed coatings region. SEM imaging was performed.

Table 1. Phosphate manganese coatings deposited at different electrolyte temperatures in naturally aerated 3% NaCl solution corrosion characteristics

Electrolyte temperature, °C	E_{corr}, mV (Ag / AgCl)	I_{corr}, µA/cm^2	β_a, mV/dec	β_c, mV/dec
20	**-1268**	**119.1**	**15.1**	**37.7**
40	**-1293**	**69.7**	**10.6**	**36.2**
60	**-1291**	**48.9**	**12.9**	**59.7**
80	**-1281**	**52.9**	**15.3**	**48.2**

Short-term (Tafel slope, Table 1) and long-term corrosion test (12 and 48 hours) were carried out. Corrosions potential stabilization first experienced phosphate manganese coatings deposited at 20 °C ASME (–900 mV), followed by 60 °C ASME (–1120 mV), 40 °C ASME (–1140 mV) and 80 °C ASME (–1210 mV).

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SYNTHESIS AND FUNCTIONALIZATION OF ZNO TETRAPOD NETWORKS FOR NEUROMORPHIC COMPUTING AND CHEMORESISTIVE SENSING SYSTEMS

Mindaugas Ilickas*, Patricija Kirvelaitytė, Martynas Tichonovas, Simas Račkauskas

Institute of Materials Science, Kaunas University of Technology, Kaunas, Lithuania
** mindaugas.ilickas@ktu.lt*

Zinc oxide (ZnO) nanoparticles are widely recognised for their low cost, low toxicity and environmental friendliness, and have attracted significant attention for applications in sensing, catalysis, optoelectronics and energy-related technologies. Among the various ZnO morphologies, ZnO tetrapods (ZnO-Ts) are particularly distinctive due to their four-armed architecture emanating from a central core, which provides high surface area, mechanical stability and efficient charge-transport pathways. These structural advantages make ZnO-T networks promising building blocks for advanced functional and neuromorphic systems.

In this work, we present a scalable and reproducible synthesis strategy for high-yield production of ZnO-Ts, together with approaches for their controlled functionalisation to enhance interfacial compatibility and application-specific performance. We investigate growth mechanisms and establish relationships between synthesis conditions, structural distributions arising from packing behaviour, and resulting electrochemical properties, providing a basis for optimising ZnO-based materials for electrocatalysis, energy storage and related applications. Furthermore, by exploiting low-temperature deposition techniques, we demonstrate that ZnO-T networks can be integrated onto virtually any substrate with controllable morphologies, enabling highly flexible device architectures.

Motivated by the increasing demands of Artificial Intelligence and the Internet of Things, which require energy-efficient hardware capable of overcoming the limitations of conventional Von Neumann architectures, we further explore ZnO-T networks as a scalable platform for neuromorphic computing and chemoresistive gas sensing. The resulting devices exhibit tunable performance via control of tetrapod size, interelectrode spacing, layer thickness and surface functionalisation. Notably, the networks demonstrate stable and repeatable optoelectronic switching behaviour, including modulation by 1 µs UV light pulses, enabling 3-bit neuromorphic memory operation that mimics synaptic weight updates.

Overall, this study establishes ZnO tetrapod networks as a versatile, low-cost and sustainable material platform for multifunctional electronics, bridging sensing, memory and optoelectronic functionality. The demonstrated integration of scalable fabrication, optical modulation and structure – property control provides a robust foundation for next-generation brain-inspired computing systems and autonomous smart devices.

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SOXHLET EXTRACTION IN THE PRODUCTION OF DIGESTATE EXTRACTS

Eglė Didžiulytė*, Rasa Šlinkšienė

Department of Physical and Inorganic Chemistry, Kaunas University of Technology, Kaunas, Lithuania
* *egle.didziulyte@ktu.lt*

Climate change encourages the search for sustainable and environmentally friendly solutions to waste management, thus adhering to the principles of the circular economy [1]. The generation of organic waste is an integral part of human activity, therefore, as the population and consumption grow, the amount of various waste is also constantly increasing [2]. Sustainable farming methods, including organic farming, are increasingly being applied in agriculture. One of the solutions being investigated and promoted is the use of digestate in agricultural soils. In the process of biogas production, microorganisms decompose organic matter of animal and plant origin under anaerobic conditions. This process produces processed biomass, called digestate.

The quality and chemical composition of the resulting digestate depends on the raw materials used in biogas production. Digestate is a valuable organic fertilizer that enriches the soil microbiota, improving its preservation and regeneration. Due to this property, it can be a satisfactory alternative to mineral fertilizers [3]. Since the digestate is rich in organic matter, digestates from various Lithuanian companies were selected for the study: “Agaro riešutas” (Biržai), “Tvari energija” (Vievis) and “Kurana” (Pasvalys). First, the concentration of organic carbon in different initial digestates was determined. The samples were dried at 60 ℃, divided into two parts, one part of which was ground. In this way, six different samples were prepared: ground and unground digestates from the three companies mentioned above. The results of the study show that the organic carbon content in the ground digestate samples ranged from 34.8 to 45.2%, and in the unground ones from 39.0 to 50.0%.

The aim of the study was to obtain the highest possible concentration of organic carbon in digestate extracts, therefore the Soxhlet extraction method was used. The extracts were produced using water and potassium hydroxide solutions (0.1 M and 0.5 M), applying the experimental conditions of the research. The samples were extracted at 3, 6 and 9 hours of boiling point. The highest organic carbon concentration was found in the potassium alkali-based extracts. It was also observed that higher potassium concentrations had a positive effect on the organic carbon content of the samples.

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THE INFLUENCE OF INDUSTRIAL OIL SHALE ASH AS A PARTIAL BINDER REPLACEMENT ON THE PROPERTIES OF AUTOCLAVED AERATED CONCRETE

Vytautas Taurele*, Raimundas Siauciunas

Department of Silicate Technology, Kaunas University of Technology, Kaunas, Lithuania
** vytautas.taurele@ktu.edu*

Autoclaved Aerated Concrete (AAC) is a widely used, highly porous building material known for its excellent thermal insulation and lightweight properties. Traditionally, the production of AAC relies on ordinary Portland cement (OPC) and lime as the main sources of calcium oxide (CaO). To address this, UAB Bauroc investigated partially replacing these binders with industrial oil shale ash (OSA) from Enefit Industry AS (Estonia). This applied research focuses on circular economy principles to minimize the environmental footprint of building materials.

The study evaluated replacing the traditional dry mix with OSA up to a maximum substitution level of 42% by mass. Since OSA contains active components like free calcium oxide (CaO_{free}) and reactive silica (SiO_2), it functions as an active binder rather than a passive filler [1]. To ensure optimal hydrothermal synthesis, mixture recipes were mathematically adjusted for each substitution level to maintain a constant total CaO content of 24% by solid mass, aligning with scientific literature [2].

Specimens were tested according to EN 772-13 and EN 772-1 standards. Quantitative X-ray diffraction (QXRD, “Rigaku MiniFlex600-C“) analysis revealed that at maximum ash integration, amount of crystalline 1.13 nm tobermorite increased from 36% to 38%. Crucially, the material maintained a dry density of 400 kg/m^3 and a compressive strength of 2.2 MPa, meeting the technical specifications of the Bauroc Roclite product line and EU standards.

These results confirm that a dynamic recipe adjustment model allows a significant portion of traditional binders to be replaced with ash while enhancing the concrete's long-term durability [3]. Ultimately, this approach successfully reduced OPC demand by approximately 59%, demonstrating a viable industrial pathway for UAB Bauroc to lower production costs and CO_2 emissions without sacrificing structural performance.

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SYNTHESIS OF 5-AMINOSALICYLIC HYDRAZIDE DERIVATIVES

Kazimieras Anusevičius*, Augustas Kučinskas, Vytautas Mickevičius

Department of Organic Chemistry, Kaunas University of Technology, Kaunas, Lithuania

* kazimieras.anusevicius@ktu.lt

The increasing majority of antibiotic-resistant bacterial infections is a major global health challenge. In particular, MRSA infections remain difficult to control, as no effective new class of antibiotics has yet been developed [1]. Therefore, the identification of alternative bacterial targets is considered essential to increase the efficacy of existing treatments and support the development of new drugs [2]. Previous studies have shown that 5-aminosalicylic acid and its derivatives can modulate bacterial growth and exhibit antibacterial activity, including against MRSA [3, 4]. In order to expand the synthetic potential, the compounds are often functionalized with hydrazide [5–7].

In this study, 5-aminosalicylic acid (1) was chosen as the starting compound for the synthesis of novel hydrazide derivatives 5a–i, as shown in Fig. 1.

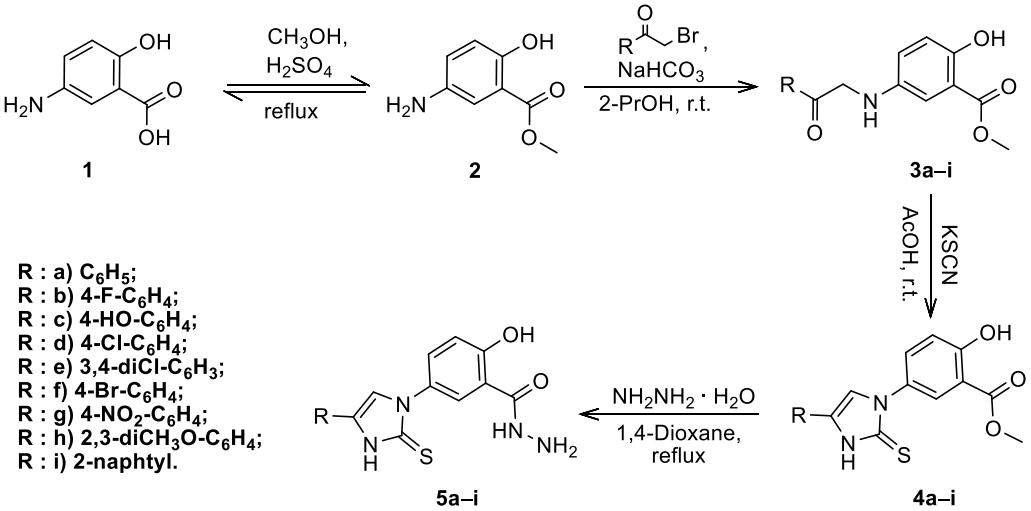

Fig. 1. The scheme of synthesis of 5-aminosalicylic hydrazide derivatives 5a–i

Initially, 5-aminosalicylic acid was esterified by the Fischer esterification method to give ester 2. Subsequently, the resulting ester was alkylated with various bromoacetophenones to give derivatives 3a–i. Compounds 3a–i were converted to imidazole derivatives 4a–i by treatment with potassium thiocyanate in acetic acid. In the final step of the synthesis, the ester functional group of the 5-aminosalicylic acid derivatives was hydrazinolysed with hydrazine monohydrate to afford the target hydrazide derivatives 5a–i.

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DEVELOPMENT OF A PEDOT:PSS-BASED, MULTILAYERED MOLECULARLY IMPRINTED ELECTROCHEMICAL SENSOR FOR TETRACYCLINE DETECTION

Beatričė Kulikauskaitė[1]*, Domas Pirštelis[1,2], Ernestas Brazys[1,2], Vilma Ratautaitė[2], Antanas Zinovičius[2], Arūnas Ramanavičius[1,2]

[1] Department of Physical Chemistry, Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Vilnius, Lithuania
[2] Department of Nanotechnology, State Research Institute Center for Physical Sciences and Technology, Vilnius, Lithuania
** beatrice.kulikauskaite@chgf.stud.vu.lt*

The widespread use of antibiotics such as tetracycline has resulted in persistent residues in the environment; therefore, given their frequent occurrence and adverse effects on living organisms, the development of effective monitoring, detection, and removal methods is of great importance. Against this background, sensors based on molecularly imprinted polymers (MIPs) are regarded as promising analytical platforms owing to their robustness, low cost, and ease of use in the detection of various analytes [1,2]. The introduction of interfacial underlayers, such as self-assembled monolayers, between the electrode and the MIP layer enables tuning of MIP properties [3].

In this work, a multilayered MIP sensor was constructed on a screen-printed carbon electrode (SPCE) platform. The SPCE was modified by drop-casting a poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS) mixture as an underlayer to tune charge-transfer characteristics. Subsequently, a molecularly imprinted polypyrrole (MIP-Ppy) layer, using tetracycline as the template, was electrochemically synthesized on the PEDOT:PSS/SPCE surface. A non-imprinted polypyrrole (NIP-Ppy) layer was prepared under identical conditions to demonstrate imprinting selectivity. The rebinding of tetracycline to the MIP/PEDOT:PSS/SPCE sensor was carried out in an acetate medium and was evaluated using electrochemical impedance spectroscopy. The constructed sensor enabled the detection of tetracycline at micromolar concentrations. The proposed multilayered, easy-to-fabricate, MIP-based electrochemical sensor demonstrates promising potential for application in the environmental monitoring of antibiotic residues.

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TEXTILE ASH WASTE AS A SUSTAINABLE METERIAL FOR THE PARTIAL REPLACEMENT OF CEMENT

Raimonda Kubiliūtė*, Evelina Švedaitė

Department of Silicate Technology, Kaunas University of Technology, Kaunas, Lithuania,
** raimonda.kubiliute@ktu.lt*

Population growth has driven rising demand and production in the textile industry. Synthetic fiber production has increased more than sixfold over the past forty years [1,2]. As a result, the textile industry contributes to environmental pollution, including water contamination from dyeing and finishing processes, air pollution from manufacturing emissions, and solid waste generation from production residues [3]. Because the textile industry generates large amounts of waste that harm the environment, recent studies have explored converting textile waste into a renewable energy source [4]. However, this process also generates secondary waste, such as textile ash. To address the environmental impacts of textile waste while meeting the growing demand for sustainable building materials, ash derived from burned textile waste has been investigated for use in cementitious materials.

In this research, a CEM I 42.5R and textile ash waste (TAW) generated by combustion of torrefied textile fuel pallets (950 °C; 1 h) were used. TAW composition consists of non-crystalline structure carbon (87.95%), calcium oxide (up to 5%), titanium oxide (4.35%), sulfur oxide (1.84%), and silicon oxide (1.15%). The ash was used as a partial replacement for ordinary Portland cement (OPC) at 0, 2.5, 5, and 7.5% by weight. Prepared cube samples (3 × 3 × 3 cm) were kept in molds for 24 hours at 23 ±2 °C, then transferred to a water bath at 25 °C for 1 day, 27 days, and 3 months. Post-hardening, compressive strength measurements were taken and XRD, VTA, SEM and CO_2 absorption data were analyzed.

It was determined that TAW particles act as a fine filler (90% of all particles have diameters up to 38.56 µm) in the cement matrix, resulting in reduced void content in the cement stone. They act as a crystallization center for nucleation of compounds and increase the density of the structure. As the TAW content increased from 2.5 to 7.5 wt.%, the compressive strength of all specimens after 28 days of curing was higher than that of OPC (77 MPa), with the highest compressive strength observed in cement specimens containing 5 wt.% TAW (88 MPa). After 3 months of hydration, the compressive strength of specimens with 7.5 wt.% TAW, possibly due to more intense CO_2 absorption (~11 % compared to pure OPC), is 1.8 % lower than that of OPC (93 MPa). The formation of a higher $CaCO_3$ content on the surface of cement particles slows calcium silicate hydration in deeper layers, thereby reducing the formation of portlandite and CSH. Thus, without compromising the properties of the cement paste, the TAW additive in cement mixtures can constitute up to 5 wt.%.

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SUSTAINABLE SYNTHESIS OF ANTIBACTERIAL CALCIUM-DEFICIENT HYDROXYAPATITE COMPOSITES FROM PHOSPHOGYPSUM WASTE

Elzbieta Jursene[1]*, Akvile Laurykietyte[1], Rokas Žalneravičius[2], Inga Grigoraviciute[1], Audrius Padarauskas[1], Aivaras Kareiva[1]

[1]Institute of Chemistry, Vilnius University, Vilnius, Lithuania
[2]Centre for Physical Sciences and Technology, Vilnius, Lithuania
** elzbieta.jursene@chgf.vu.lt*

The continuous accumulation of phosphogypsum (PG), a by-product of phosphoric acid manufacturing, represents a significant environmental challenge. At the same time, the development of cost-efficient biomaterials with antibacterial properties is of growing importance in bone tissue engineering. This study explores a sustainable approach to address both issues by converting PG into calcium-deficient hydroxyapatite (CDHA) composites functionalized with malachite green (MG), a compound known for its antimicrobial activity.

PG obtained from the Lifosa industrial facility (Kedainiai, Lithuania) was used as the primary calcium source for CDHA formation. MG was incorporated during synthesis to provide antibacterial functionality. The structural and physicochemical properties of the prepared composites were investigated using X-ray diffraction, field-emission scanning electron microscopy (FE-SEM), high-performance liquid chromatography (HPLC), and thermogravimetric–differential scanning calorimetry (TG-DSC).

The results revealed that synthesis conditions significantly affect the phase composition and thermal stability of the obtained materials. TG-DSC analysis demonstrated multiple thermal events associated with the decomposition of both organic and inorganic components, confirming the complex, multiphase nature of the composites. HPLC data verified the successful incorporation of MG into the apatite structure, while FE-SEM analysis provided insight into the morphology and microstructure of the materials.

The findings highlight the potential of PG as a low-cost raw material for the production of antibacterial bioceramics. This approach contributes to circular economy principles by enabling the valorization of industrial waste into functional materials suitable for applications in bone regeneration and infection control.

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EFFECT OF SYNTHESIS ROUTE ON CALCIUM-DEFICIENT HYDROXYAPATITE COMPOSITES INCORPORATING PROPOLIS POWDER

Justina Karciauskaite[1]*, Maab Elsheikh[1], Rokas Zalneravicius[2,3], Inga Grigoraviciute[1], Zivile Stankeviciute[1], Aivaras Kareiva[1,]

[1]Institute of Chemistry, Vilnius University, Vilnius, Lithuania,
[2]Center for Physical Sciences and Technology, Vilnius, Lithuania,
[3]Institute of Biochemistry, Life Sciences Center, Vilnius University, Vilnius, Lithuania,
* *justina.karciauskaite@chgf.stud.vu.lt*

Calcium-deficient hydroxyapatite (CDHA; $Ca_9(HPO_4)(PO_4)_5OH$) is a biomimetic material widely recognized for its similarity to the mineral phase of human bone, making it a promising candidate for biomedical applications [1,2]. Propolis is a naturally occurring resinous substance harvested by honeybees (*Apis mellifera*) from the buds and leaves of various plant species, which is subsequently combined with bee wax [3,4]. In this study, CDHA–propolis composites were synthesized using propolis in powder form via both ex-situ (mechanical mixing) and in situ (precipitation-assisted incorporation) approaches at concentrations ranging from 2.5 to 10 wt%. The effect of synthesis route and propolis content on the physicochemical properties of the composites was systematically investigated. Structural and compositional characterization was carried out using X-ray diffraction (XRD), Fourier-transform infrared (FTIR) spectroscopy, thermogravimetric analysis (TG), scanning electron microscopy (SEM), and Brunauer–Emmett–Teller (BET) surface area analysis. XRD results confirmed the formation of phase-pure CDHA in all samples. FTIR analysis revealed characteristic organic bands corresponding to propolis constituents, indicating successful incorporation into the CDHA matrix. SEM observations showed that in situ incorporation of propolis powder led to more uniform particle distribution and reduced particle size compared to ex situ mixing. Thermogravimetric analysis demonstrated increased organic content with higher propolis loading. Additionally, BET measurements indicated a decrease in specific surface area with increasing propolis concentration, suggesting partial pore blocking and particle agglomeration. Overall, the findings highlight the significant influence of synthesis route and propolis powder incorporation on the structural and physicochemical properties of CDHA-based composites, supporting their potential as antibacterial agents. Moreover, for further development in biomedical applications.

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HER AND OER BEHAVIOR OF DIFFERENT Au(NiZn)/Ti BASED ELECTROCATALYSTS

Tripura Ganti*, Aldona Balčiūnaitė, Jūrate Vaičiūnienė, Loreta Tamašauskaitė-Tamašiūnaitė, Eugenijus Norkus

Department of Catalysis, Center for Physical Sciences and Technology, Vilnius, Lithuania
** tripura.ganti@ftmc.lt*

Electrochemical water splitting has been identified as a sustainable approach for hydrogen production, wherein the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER) play crucial roles. However, OER suffers from sluggish kinetics, particularly due to the multi-step OER process, which limits the overall efficiency of water splitting systems. Thus, the development of efficient and stable electrocatalysts is essential to reduce overpotential and enhance reaction rates in alkaline media.

Nickel (Ni)-based materials have gained significant interest as promising electrocatalysts due to their cost-effectiveness, excellent electrical conductivity, and ideal catalytic properties. In particular, NiZn-based systems offer a tunable electronic structure and surface properties, which can be further optimized through techniques such as leaching and noble metal integration. Leaching can selectively remove less active components, leading to increased surface area and exposure of catalytically active sites, thereby enhancing HER performance. On the other hand, the incorporation of noble metals such as Au can significantly improve OER activity by modulating the electronic structure and facilitating reaction kinetics.

In the present study, a NiZn catalyst was fabricated via electrodeposition on a Ti substrate. This was then subjected to selective leaching in 1 M KOH for a period of 24 hours to obtain a leached NiZn/Ti catalyst, and Au was incorporated onto the unleached NiZn/Ti catalyst via a galvanic displacement process. The structural and morphological properties of the prepared electrodes were characterized using X-ray diffraction and scanning electron microscopy. The elemental composition and metal loading of the catalysts were determined by inductively coupled plasma optical emission spectroscopy. Furthermore, chronoamperometry was conducted to evaluate the stability of the electrocatalysts. Overall, this study demonstrates that surface leaching significantly enhances HER activity by increasing active surface sites. In contrast, the incorporation of Au improves OER performance by promoting favorable electronic interactions and reaction kinetics.

FROM WASTE TO TREASURE: NEO-CYCLE APPROACH TO CONVERT E-WASTE INTO VALUABLE MATERIALS

Gintarė Sujetovienė, Jūratė Žaltauskaitė, Diana Miškelytė, Renata Dagiliūtė*

Vytautas Magnus University, Kaunas reg., Lithuania
* *renata.dagiliute@vdu.lt*

The transition toward sustainable and circular chemical technologies is a defining challenge for modern research and industrial development. A strategic priority within this shift is the advancement of separation science to improve the recovery and functional reuse of Critical Raw Materials (CRMs). Currently, the chemical industry faces a dual imperative: securing a stable supply of strategic elements while mitigating the environmental footprint of hazardous electronic waste. Demand for Nd is projected to double by 2030 and increase sevenfold by 2040, driven by the mass production of electric vehicle motors and wind turbines [1]. Despite this demand, the EU remains over 90% dependent on external suppliers for processed REEs, with a single country controlling approximately 85% of global processing capacity [2]. To mitigate this vulnerability, the EU Critical Raw Materials Act (CRMA), which entered into force in 2024, sets a 2030 target for at least 25% of the EU's annual demand for strategic raw materials to be covered by recycling capacity [3].

Despite their importance, the recycling rates of Rare Earth Elements (REEs) remain critically low – often below 1% - particularly from complex wastes such as hard disk drives. Neodymium-iron-boron (NdFeB) magnets represent a highly concentrated but underutilized source of REEs. The NEO-CYCLE project directly addresses this "recovery gap" by demonstrating a high-TRL pathway to reclaim high-purity Nd, Fe, and B from magnet waste, transforming a supply chain liability into a strategic resource for European industry. This approach integrates advanced chemical recovery and separation technologies to transform waste into high quality secondary raw materials. Core processes include solid-state chlorination, selective electrochemical extraction of neodymium, and advanced purification techniques to achieve market-grade purity levels for Nd, Fe, and B. The recovered elements are further upcycled into high-value functional products with targeted industrial applications, ensuring properties and performance comparable to those derived from primary raw materials. These materials are to be used in pharmaceutical manufacturing, including catalysts for active pharmaceutical ingredient (API) synthesis, as well as in ammonia production for fertilizers. In addition, they are applied as catalysts in polymer development and as nanoparticle-based systems for advanced catalytic processes, including green ammonia synthesis. Overall, the project results demonstrate the significant potential of electronic waste as a source of strategic materials for the pharmaceutical, fertilizer, and polymer sectors. This work supports enhanced resource efficiency, reduced environmental impact, and the development of technologies for resilient circular chemical industry, converting waste back into useful products.

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ADSORPTION–DESORPTION OF CR(III) AND CR(VI) ON SUSTAINABLE BUCKWHEAT HULL BIOSORBENT: ISOTHERM, KINETICS AND THERMODYNAMIC EVALUATION

Tayyab Tahir[1]*, Rūta Druteikienė[1], Zita Žukauskaitė[1], Rūta Barisevičiūtė[1], Jūratė Vaičiūnienė[2]

[1] Department of Nuclear Research, Center for Physical Sciences and Technology Savanorių ave. 231, LT-02300 Vilnius, Lithuania
[2] Department of Catalysis, Center for Physical Sciences and Technology Saulėtekio av. 3, LT-10257 Vilnius, Lithuania
** tayyab.tahir@ftmc.lt*

Large volumes of industrial wastewater from leather, metallurgy, and electroplating industries contribute significantly to chromium contamination in aquatic environments. Chromium mainly exists as Cr(III) and Cr(VI), of which Cr(VI) is highly toxic due to its carcinogenic, mutagenic, and teratogenic effects. The presence of Cr(VI) poses serious risks to human health and environmental safety, necessitating its effective removal from wastewater. [1]. Therefore, it is crucial to invent cost effective and safe treatment methods to keep water clean. In recent times, these toxic metals have been separated from water through reverse osmosis, electrochemical processing, redox processes, membrane separation, ion exchange precipitation. Adsorption is widely recognized as a environmentally sustainable and cost-effective technique for heavy metal removal, offering significant advantages such as high efficiency and selective binding of metal ions even at low concentrations [2].

The present study investigates the removal of Cr(III) and Cr(VI) from an aqueous solution by using buckwheat hull as a biosorbent. The experimental parameters encompass temperature (25–50 °C), solution pH (2-7), the amount of buckwheat hull (0.1–0.35 g), the initial Cr(III/VI) concentration (5–200 mg L^{-1}), and the contact time (30–1440 min). SEM, FT-IR, EDX, BET and pH of point of zero charge (pH_{pzc}) were applied for the characterization of biosorbent. The sorption depends on pH and maximum sorption of Cr(III) and Cr(VI) was acquired at pH 5 and 2, respectively. Kinetics models (as pseudo-first-order, pseudo-second-order, intraparticle diffusion and Elovich) were applied in the study of sorption data. The pseudo-second-order kinetic model yielded higher agreement with experimental results in comparison to the pseudo-first-order kinetic model due to the higher values of R^2=0.999 for both metal ions Cr(III) and Cr(VI), indicating that chemisorption is the dominant mechanism. The isotherm study was conducted with the implementation of four models: Langmuir, Freundlich, Dubinin Radushkevich (D-R), and Temkin isotherms. The equilibrium data of Cr(III) and Cr(VI) was found to follow the Langmuir model which show the monolayer adsorption. Desorption and regeneration studies demonstrated that buckwheat hull can be effectively reused over multiple cycles with acceptable efficiency. Overall, the results highlight that buckwheat hull is an efficient, sustainable, and cost-effective biosorbent for the removal of chromium from aqueous systems.

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SPIRO[1,3-DITHIOLANE-2,9'-FLUORENE]- AND DIBENZOTHIOPHENE-BASED HOLE TRANSPORTING MATERIALS FOR PHOTOVOLTAIC APPLICATIONS

Adnan Ahmed[1]*, Nagharsh Mirakyan[1], Asta Dabuliene[1], Edwin Pineda De La O[2], Dmytro Volyniuk[1], Oleksandr Bezvikonnyi[1], Lethy Krishnan Jagadamma[2], Juozas Vidas Grazulevicius[1]

[1] Department of Polymer Chemistry and Technology, Kaunas University of Technology, Kaunas, Lithuania
[2] University of St Andrews, School of Physics and Astronomy, Energy Harvesting Research Group, SUPA, Scotland
* *adnan.ahmed@ktu.edu*

Organic hole-transporting materials (HTMs) are key components in perovskite solar cells (PSCs), governing charge extraction, recombination, and device stability [1,2]. Widely used HTMs such as spiro-OMeTAD and PTAA provide high performance but their application is limited by high cost, low intrinsic mobility, complex synthesis and stability issues [3,4].

To address these limitations, two new hole-transporting compounds with the same side donor moiety and the different central fragments, i.e., those of dibenzothiophene or spiro[1,3-dithiolane-2,9'-fluorene] were designed and synthesyzed using microwave irradiation-assisted Buchwald–Hartwig cross-coupling reactions. Atomic force microscopy revealed average surface roughness values in the range of 6.13–8.03 nm, a parameter relevant to interfacial charge transport. Thermal analysis showed high thermal robustness, with the temperatures of the onsets of thermal degradation exceeding 300 °C and glass transition temperatures reaching up to 163 °C. The solid films of the compounds are characterised by low ionisation energies of ca. 5.0 eV. According to charge extraction by linearly increasing voltage (CELIV) and time-of-flight experiments, the spiro[1,3-dithiolane-2,9'-fluorene] derivative exhibits hole mobility reaching 1.8×10^{-4} $cm^2/V\cdot s$ at electric field of 3.17×10^5 V/cm. When the spiro[1,3-dithiolane-2,9'-fluorene] derivative is used for the deposition of hole-transporting layers, perovskite solar cells achieve maximum power conversion efficiencies of 15.5% under solar illumination and 30% under indoor illumination, demonstrating the superior potential of spiro[1,3-dithiolane-2,9'-fluorene] derivatives over dibenzothiophene derivatives in molecular structure design.

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COMPARATIVE PHYSICOCHEMICAL AND MORPHOLOGICAL CHARACTERIZATION OF SPENT COFFEE GROUNDS AND BIOCHAR AS ADDITIVES FOR GYPSUM BINDER

Nora Kybartienė[1]*, Neringa Matutytė[1], Vydmantė Astrauskaitė[1], Irena Vaškevičienė[2], Simona Tučkutė[3]

[1] Faculty of Chemical Technology, Kaunas University of Technology, Kaunas, Lithuania
[2]Laboratory of Heat-Equipment Research and Testing, Lithuanian Energy Institute,Kaunas, Lithuania
[3]Center for Hydrogen Energy Technologies, Lithuanian Energy Institute, Kaunas, Lithuania
* *nora.kybartiene@ktu.lt*

As the building materials industry moves towards a circular economy model, the assessment of organic waste and its use as sustainable additives is becoming increasingly relevant [1]. Coffee is one of the most widely consumed beverages in the world, resulting in huge amounts of spent coffee grounds (SCG) being generated every year. The ever-growing amount of this waste poses a serious environmental challenge, so it is necessary to find solutions to use them [2]. One of the promising solutions is to incorporate SCG and SCG-derived biochar into the gypsum binder. In order to ensure the structural integrity of the gypsum matrix and its suitable performance properties, a detailed analysis of the chemical composition and crystal morphology of the waste is required.

The aim of this study is to perform a comparative analysis of the physical, chemical and morphological properties of spent coffee grounds (SCG) and biochar derived from SCG with the aim of reusing them in the production of gypsum binders.

SCG was collected from a local coffee shop and dried at 80 °C. Biochar was prepared by heating SCG at 320 and 500 °C in an oxygen-limited atmosphere for two hours.

The materials were characterized by various methods. The elemental composition was determined using X-ray fluorescence (XRF) and CHNX analysis. Crystallinity was determined using X-ray diffraction (XRD), thermal stability was assessed by simultaneous thermal analysis (STA), and functional groups were analyzed using Fourier transform infrared spectroscopy (FTIR) and morphological analysis was performed using scanning electron microscopy (SEM). The pH, moisture content, specific surface area and density of the materials were determined.

The results provide a basis for explaining the different effects of spend coffee ground and biochar on the physical-mechanical properties of gypsum binders.

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NOVEL 3-(DIPHENYLAMINO)CARBAZOLE EMITTERS FOR MULTI-CHANNEL GREEN TADF OLEDS

Raminta Beresneviciute[1]*, Inesa Sasnauskaite[2], Zeyad Taher Abdou[1], Dovydas Blazevicius[1], Saulius Grigalevicius[1], Wanting Ju[2], Xiangqin Gan[2], Junqiao Ding[2], Kaspars Traskovskis[3]

[1] Department of Polymer Chemistry and Technology, Kaunas University of Technology, Kaunas, Lithuania
[2] School of Chemical Science and Technology, Yunnan University, Kunming, P. R. China
[3]Faculty of Natural Sciences and Technology, Riga Technical University, Riga, Latvia
** raminta.beresneviciute@ktu.lt*

High-performance thermally activated delayed fluorescence (TADF) emitters are currently in great demand for applications in full-color displays and solid-state lighting. These materials can reach up to 100% internal quantum efficiency (IQE) without relying on noble metals. TADF effect enables the upconversion of triplet excitons into emissive singlet states through reverse intersystem crossing (RISC), provided that the singlet-triplet energy gap (ΔE_{ST}) is sufficiently small, and for this goal, a good spatial separation between HOMO and LUMO orbitals is required, which is typically accomplished by incorporating both donor and acceptor moieties into a single molecule using donor-acceptor or donor-acceptor-donor architectures [1-3]. In this study, a new series of 3-(diphenylamino)carbazole-based compounds, RB91, RB92, and RB93, was successfully synthesized and investigated. The structures of materials are shown in Fig. 1.

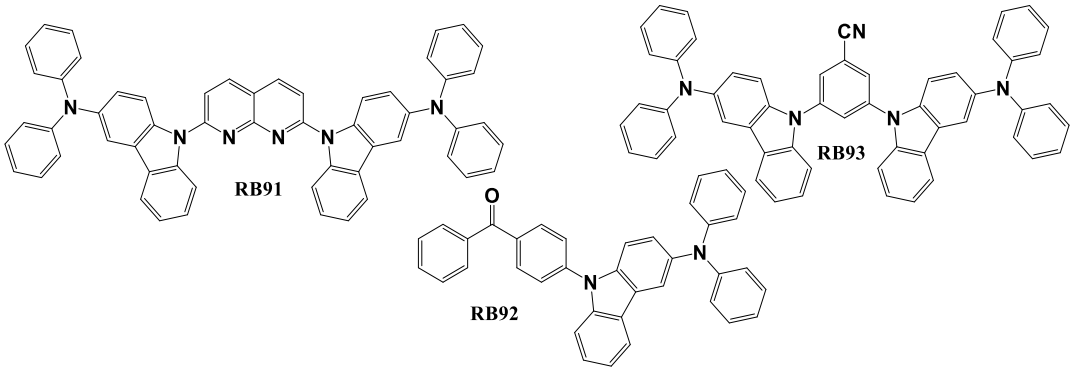

Fig. 1. Chemical structures of 3-(diphenylamino)carbazole-based derivatives

All compounds exhibited green photoluminescence and TADF with microsecond-range delayed lifetimes. Twelve OLED prototypes were fabricated using these emitters. RB91 emerged as the top performer, achieving a peak EQE of 12.87% and the highest current/power efficiencies (37.24 cd/A, 41.34 lm/W). The observed performance is attributed to the small ΔE_{ST} (0.14 eV) and its optimized excited-state characteristics, enabling efficient RISC and low efficiency roll-off at high brightness.

Acknowledgements. We are obliged to the Research Council of Lithuania for the support (Grant. No. S-LLT-25-2).

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MALACHITE AND VERDIGRIS PAINTS ON PAPER: A SPECTROSCOPIC STUDY OF DEGRADATION PROCESSES

Gustė Rudaitytė[1]*, Aivaras Kareiva[1], Aušra Čiuladienė[2]

[1]Department of Inorganic Chemistry, Vilnius University, Vilnius, Lithuania
[2]Documents Conservation and Restoration Department, The Wroblewski Library of the Lithuanian Academy of Sciences, Vilnius, Lithuania
** guste.rudaityte@chgf.stud.vu.lt*

Copper-based green pigments such as malachite and verdigris are historically significant materials used in artworks on paper, but their chemical instability poses serious challenges for long-term preservation [1, 2]. Copper ions present in these pigments are key contributors to the oxidative degradation of cellulose in paper-based cultural heritage objects. In particular, these Cu^{2+} ions can catalyze Fenton-type reactions, leading to the generation of highly reactive hydroxyl radicals, which cleave the β-1,4-glycosidic bonds in cellulose, resulting in degradation of the paper substrate [3].

In this study, paper samples coated with malachite and verdigris paints were subjected to accelerated aging under controlled environmental conditions. After aging, the samples were characterized using pH measurements, colorimetric analysis, and Fourier-transform infrared (FTIR) spectroscopy to evaluate chemical and structural changes occurring in both the paint layers and the paper substrate.

The accelerated aging protocol led to a decrease in pH and pronounced color changes (ΔE*), which were more evident in verdigris-containing samples. FTIR spectroscopy confirmed these observations, revealing clear spectral changes in verdigris consistent with underlying chemical transformations. Malachite demonstrated greater stability, with only minor spectral changes detected. These results suggest distinct degradation behaviors of the two copper-based paints under the applied aging conditions. Further studies using complementary analytical techniques are needed to better understand the mechanisms underlying the observed transformations.

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STRUCTURAL EVOLUTION OF $YbFe_{1-x}Mn_xO_3$ SOLID SOLUTIONS PREPARED BY SOL–GEL METHOD

Aigul Dastankyzy[1]*, Dovydas Karoblis[1], Kestutis Mazeika[2], Aivaras Kareiva[1]

[1]Institute of Chemistry and Geosciences, Vilnius University, Vilnius, Lithuania
[2]Center for Physical Sciences and Technology, Vilnius, Lithuania
* *aigul.dastankyzy@chgf.stud.vu.lt*

The rare-earth manganite $YbMnO_3$ and orthoferrite $YbFeO_3$ are complex oxides whose structural and magnetic properties are governed by distortions of BO_6 (B = Mn, Fe) coordination polyhedra in a perovskite-related lattice. These materials attract considerable interest due to their complex magnetic ordering and the strong coupling between crystal structure and physical properties [1].

$YbFeO_3$ crystallizes in an orthorhombically distorted perovskite structure (space group Pbnm) and exhibits antiferromagnetic ordering with a weak ferromagnetic component due to spin canting [2]. In contrast, $YbMnO_3$ is typically stabilized in a hexagonal structure (space group $P6_3cm$), where Mn ions form trigonal bipyramidal MnO_5 units [3]. This phase exhibits multiferroic behavior, while $YbFeO_3$ is not multiferroic under ambient conditions [4].

The structural features of intermediate compositions in the $YbFe_{1-x}Mn_xO_3$ system remain insufficiently studied. Due to the differences between the end members, partial substitution of Fe by Mn is expected to induce structural modifications and affect the system's properties.

In this work, a series of $YbFe_{1-x}Mn_xO_3$ compositions was synthesized using the sol-gel method to investigate the influence of Fe/Mn substitution on the structural characteristics of the system. Phase formation and crystal structure were studied by X-ray diffraction (XRD) and Fourier-transform infrared (FT-IR) spectroscopy. The morphology and microstructure of the samples were examined using scanning electron microscopy (SEM), while the elemental composition and chemical homogeneity were analyzed by SEM-EDX and inductively coupled plasma optical emission spectroscopy (ICP-OES). The obtained results confirm the successful synthesis of $YbFe_{1-x}Mn_xO_3$ compositions and demonstrate that Fe/Mn substitution affects the structural characteristics of the system and leads to structural transition from orthorhombic to hexagonal structure.

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IMPACT OF DENDRITIC GOLD NANOSTRUCTURES ON THE ELECTROCHEMICAL RESPONSE OF A GLUCOSE BIOSENSOR FOR CADMIUM IONS DETECTION

Katazyna Blazevic[1]*, Natalija German[2], Asta Kausaite-Minkstimiene[1,2], Almira Ramanaviciene[1,2]

[1] NanoTechnas - Center of Nanotechnology and Materials Science, Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Vilnius, Lithuania
[2]Department of Immunology and Bioelectrochemistry, State Research Institute Centre for Innovative Medicine, Vilnius, Lithuania
** katazyna.blazevic@chgf.vu.lt*

Cadmium ions (Cd^{2+}) are toxic environmental contaminants that can accumulate in living systems and pose serious health risks, highlighting the need for simple and reliable detection methods [1-2]. In this work, an electrochemical biosensor based on glucose oxidase (GOx) was used to determine Cd^{2+} ions via their inhibitory effect on enzyme activity. Detection relied on measuring the decrease in the current generated during glucose oxidation.

To improve the biosensor's analytical response to Cd^{2+}, graphite rod (GR) electrodes were modified with dendritic gold nanostructures (DAuNSs). The behavior of a biosensor based on a GR/DAuNSs/GOx electrode was evaluated and compared with that of a biosensor based on a GR/GOx electrode. In all tested configurations, exposure to Cd^{2+} reduced GOx activity and, consequently, the electrochemical signal. A pronounced inhibitory effect was observed for electrodes modified with DAuNSs. The obtained results indicate that DAuNSs improves the performance of GOx-based electrochemical biosensors for the detection of Cd^{2+} and may also be useful for sensing other toxic metal ions.

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SYNTHESIS OF CALCIUM SILICATES HARDENING IN A CO_2 ENVIRONMENT FROM SECONDARY RAW MATERIALS

Agne Anusauskaite*, Evelina Svedaite, Tadas Dambrauskas, Kestutis Baltakys

Kaunas University of Technology, Kaunas, Lithuania,
* *agne.anusauskaite@ktu.lt*

Global CO_2 emissions and industrial waste levels are increasing rapidly, posing a major environmental challenge [1]. In Lithuania, more than 2.3 million tonnes of calcium-containing industrial waste arise annually across various sectors, including agriculture, chemical production, and thermal processes, with over 95% of this waste being landfilled or otherwise disposed of [2]. Despite their significant potential to be converted into materials that harden in a CO_2 environment, these wastes remain underutilized [3-4]. In this context, the synthesis of calcium silicates from industrial waste represents a promising approach, as these materials react with CO_2, leading to carbonation and material hardening.

In this study, two industrial secondary materials were used as raw materials: a waste derived from concrete production residues (CW) and a sludge-like by-product (SW) from water treatment processes. The raw materials were dried, crushed, and ground in a rotary mill for 2 h, followed by additional grinding in a planetary mill (700-900 rpm) for 10 minutes. The prepared materials were mixed by adding SW to the CW to adjust the initial Ca/Si (C/S) ratio (≈0.87) to 1.0, 1.5, and 2.0. The mixtures were then subjected to high-temperature treatment at 700-1300 °C for 1 h. The raw materials and synthesized products were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR), X-ray fluorescence (XRF), and simultaneous thermal analysis (STA).

XRD analysis showed that both raw materials mainly consisted of calcite, quartz, and dolomite. In addition, XRF results showed that the sludge waste contains high $CaCO_3$ content (up to 76 wt.%) and the concrete-derived waste contains significant SiO_2 (30 wt.%), confirming their suitability as precursors for calcium silicate synthesis. It was determined that CW and SW are suitable materials for the synthesis of calcium silicates because the mixture of wollastonite ($CaSiO_3$), rankinite ($Ca_3Si_2O_7$), and dicalcium silicates (Ca_2SiO_4) was obtained. The composition of the obtained products depended on both calcination temperature and the molar ratio of the initial mixture. These findings demonstrate the feasibility of converting industrial waste into silicates hardening with CO_2 capture.

Acknowledgements. This research was supported by the Research Council of Lithuania under the project "Production of Innovative Solid CO_2 Binder Based on Calcium-Rich Industrial Wastes (PICOBIND)" (Project No. S-MIP-25-4).

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DERIVATIVES OF ISOPHTALOYL FOR EFFICIENT HARVESTING OF TRIPLET EXCITONS

Mariia Stanitska[1,2]*, Melika Ghasemi[2] Ugne Seibetytė[2], Dmytro Volyniuk[2], Juozas Vidas Gražulevičius[2]

[1] Centre for Physical and Technological Sciences, Vilnius, Lithuania,
[2] Kaunas University of Technology, Kaunas, Lithuania,
* *mariia.stanitska@ktu.lt*

Crystalline organic semiconductors have great potential for use in organic optoelectronic devices because they exhibit higher charge carrier mobility than their amorphous counterparts. They have highly oriented transition dipole moments and better morphological stability that is required for the development of state-of-the-art organic light-emitting diodes (OLEDs). The aim of work is the development of highly efficient and stable OLEDs using new crystallizable emitters, exhibiting thermally activated delayed fluorescence (TADF). TADF emitters are recognized as the third generation of OLED emitters with the ability to reach 100% conversion of electrically generated singlets and triplets to light. Herein, we present three novel organic luminophores based on isophtaloyl electron-accepting core, ornamented with various electron-donating moieties, such as 3,6-diphenyl-9H-carbazole, 10H-phenothiazine, 9,9-dimethyl-9,10-dihydroacridine. All the compounds were crystalline, as proved by differential scanning calorimetry and single-crystal X-ray diffraction, and highly thermally stable with decomposition temperatures exceeding 300 °C. The luminophores were characterized by high and balanced charge-carrier mobility values reaching 10-3 order of magnitude for acridine-containing compound. All the compounds are characterized by high spatial separation of frontier molecular orbitals and negligible values of singlet-triplet energy splitting, that enabled efficient utilization of triplet excitons through fast reverse intersystem crossing. Compounds were found to emit blue (9,6-diphenyl-9H-carbazole), green (9,9-dimethyl-9,10-dihydroacridine) and yellow (10H-phenothiazine) TADF. OLED based on phenothiazine-containing compound as emitting material afforded yellow electroluminescence with 20% of external quantum efficiency.

Acknowledgements. This project has received funding from the Europen Union in frame of Research and Innovation Strategy for Lviv Polytechnic National University dedicated to White-Emitting Organic Lighting Systems (HELIOS) project.

HYDROTHERMAL SYNTHESIS OF CALCIUM SILICATE HYDRATES WITH DOLOMITE SCREENINGS AND THEIR EFFECT ON OPC HYDRATION

Neringa Kausinyte, Tadas Dambrauskas*, Kestutis Baltakys

Department of Silicate Technology, Kaunas University of Technology, Kaunas, Lithuania,
** tadas.dambrauskas@ktu.lt*

Waste generation and recycling remain among the biggest challenges in Europe and worldwide. In 2022, more than 2.2 billion tonnes of waste were generated in the European Union, but only about 40% of it was recycled [1]. One way to use waste is in the production of more environmentally friendly binders or binder additives. This approach not only recycles waste but also helps reduce problems associated with binder production, such as high CO_2 emissions and the large consumption of natural raw materials [2]. A major challenge in using waste in binder production is the uneven composition and variable properties of waste materials, which often require additional treatment [3]. One possible method is hydrothermal treatment, during which calcium- and silica-containing waste can be converted into calcium silicate hydrates that can be used as additives to improve cement properties [4]. Therefore, the aim of this study was to use dolomite processing waste to synthesize calcium silicate hydrates and to determine the effect of the obtained products on Portland cement hydration.

Hydrothermal synthesis of calcium silicate hydrates was carried out in mixtures of calcium oxide and quartz with a CaO/SiO_2 molar ratio of 1.5, using 5 wt% and 10 wt% dolomite screenings. The solid mixtures were mixed with water at a water-to-solid ratio of 10. The suspensions were treated under hydrothermal conditions at 175–225 °C for 16–72 h. The products obtained under the most suitable synthesis conditions were then used as an additive for ordinary Portland cement (OPC), replacing 5 wt%, 10 wt%, and 15 wt% of cement. Hydration behaviour was evaluated by isothermal microcalorimetry.

The results showed that the most suitable amount of dolomite screenings in the $CaO\text{-}SiO_2\text{-}H_2O$ system was 5 wt%, and the most suitable synthesis conditions were 175 °C and 16 h of hydrothermal treatment. Increasing the amount of dolomite screenings to 10 wt% negatively affected the formation of silicates. Meanwhile, in cement mixtures, the optimal amount of the synthetic additive was up to 10 wt%, as this level promoted early-stage hydration. Additional thermal treatment of the synthetic additive had an even stronger effect on OPC hydration, as the formation of aluminate phases became more pronounced.

Acknowledgements. This research was supported by the Research Council of Lithuania under the project "Production of Innovative Solid CO_2 Binder Based on Calcium-Rich Industrial Wastes (PICOBIND)" (Project No. S-MIP-25-4)

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FRASS – A NEW SOURCE OF ORGANIC FERTILIZER

Goda Gudinskaitė*, Rasa Paleckienė

Department of Physical and Inorganic Chemistry, Kaunas University of Technology, Kaunas, Lithuania
** goda.gudinskaite@ktu.lt*

When discussing the future, edible insects are often mentioned as an important alternative source of protein for humans. More than 2,000 species of edible insects are known worldwide. The seven main insect species most commonly farmed globally are black soldier flies (*Hermetia illucens*), house flies (*Musca domestica*), mealworms (*Tenebrio molitor*), lesser mealworms (*Alphitobius diaperinus*), house crickets (*Acheta domesticus*), banded crickets (*Gryllodes sigillatus*), and Jamaican field crickets (*Gryllus assimilis*). Insect farming is considered one of the alternatives to traditional agricultural production systems [1, 2]. The insect farming sector is expanding rapidly worldwide, resulting in increasing amounts of by-products being generated. The use of these raw materials for the production of fertilizers would not only reduce waste generation but also create value-added products.

Insect-derived by-products are being studied, processed, and adapted for the development of stable and effective fertilizer products. In this way, several challenges can be addressed simultaneously: waste volumes can be reduced, more sustainable fertilizers can be developed, and dependence on traditional energy-intensive products can be decreased.

In this study, waste (Frass) generated during cricket (Acheta domestic) farming by the company UAB "Eurocrickets" was analyzed and its chemical composition was determined (Table 1). Several different batches of Frass (SF1, SF2) were evaluated for their suitability for fertilizer production. The concentration of organic matter in the frass samples was determined to be about 90% (w/w).

Table 1. Chemical composition of cricket (Acheta domestic) Frass

Samples	N, %	P_2O_5, %	K_2O, %	Organic carbon (C), %	Humic acid content, %	Fulvic acid content, %
SF1	3.64	1.58	0.72	25.66	0.59	0.59
SF2	3.84	2.10	0.85	25.94	0.15	0.16

Extracts were produced from this waste under different conditions to isolate biologically active substances. Optimal processing conditions were identified, and the stability of the obtained extracts was studied. Continuing the research, extracts obtained from insect farming waste were formulated with liquid complex fertilizers. Micro vegetative studies were conducted to assess the agrochemical efficiency of the resulting products. The results indicate that the newly developed components can be successfully integrated into fertilizer products and have a positive effect on plants. Consequently, this raw material has the potential to become a part of innovative fertilizers.

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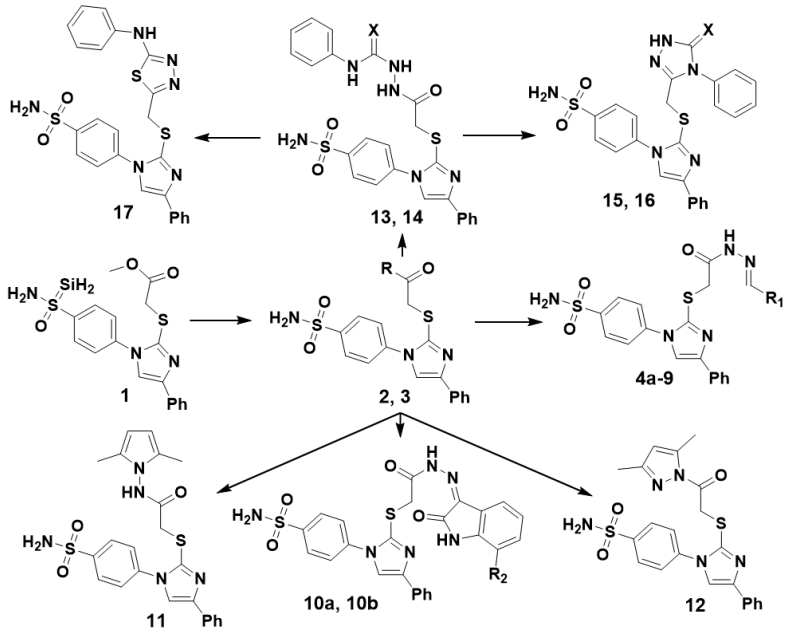
SYNTHESIS AND BIOLOGICAL EVALUATION OF 2-MERCAPTOIMIDAZOLES BEARING HYDRAZONE, AZOLE AND BENZENESULFONAMIDE MOIETIES

Valdas Vainauskas[1]*, Vytautas Mickevičius[1], Birutė Grybaitė[1], Kotryna Čiupkevičiūtė[2], Vilma Petrikaitė[2]

[1]Kaunas University of Technology, Department of Organic Chemistry, Kaunas, Lithuania
[2]Department of Drug Targets Histopathology, Institute of Cardiology, Lithuanian University of Health Sciences
** valdas.vainauskas@ktu.edu*

In this study, a series of novel S-alkylated imidazole derivatives 1-17, bearing a sulfonamide moiety, were synthesized. The ester group of starting material was utilized to produce compounds 2,3 bearing hydrazide and hydroxamic acid moieties. Furthermore, hydrazide 3 was successfully exploited in synthesis of various aromatic and heterocyclic hydrazones 4a-10b, semicarbazides 13, 14 and azoles 11, 12, 15-17 (Fig. 1.).



1 R = OCH_3; **2** R = NHOH; **3** R = $NHNH_2$; **4a** R_1 = C_6H_5; **4b** R_1 = 4-ClC_6H_4; **4c** R_1 = 4-FC_6H_4; **4d** R_1 = 2-$H_3COC_6H_4$; **4e** R_1 = 2-HOC_6H_4; **5** R_1 = 1-naphthyl; **6** R_1 = 3-thienyl; **7a** R_1 = 5-bromo-2-thienyl; **7b** R_1 = 5-nitro-2-thienyl; **8** R_1 = pyrrol-2-yl; **9** R_1 = pyridin-4-yl; **10a** R_2 = H; **10b** R_2 = Br; **13, 15** X = S; **14, 16** X = O;

Fig. 1. Synthesis of various 2-mercaptoimidazole derivatives

Compounds were tested against human prostate carcinoma PC3, triple-negative breast cancer MDA-MB-231, and glioblastoma U-87 cell lines, under normoxia and hypoxia. The effect on cell viability was determined by the MTT assay at 20 μM of compounds after 72 hours of incubation.

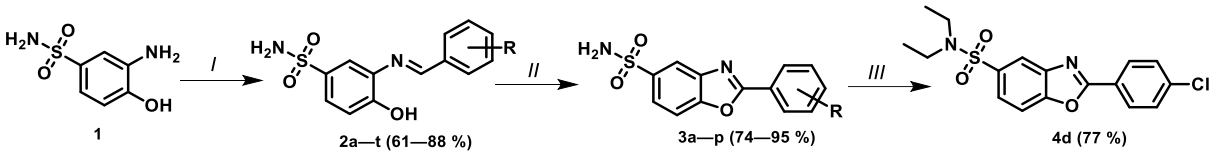
Compounds 1, 4a, 4b, 4c, 7a, 7b and 12 reduced the viability of all cell lines by up to appr. 20-25% and were identified as the most active ones. The greatest difference in activity under normoxia and hypoxia conditions was determined in the MDA-MB-231 cell line, especially for compounds 4a, 4b, and 7b. Compound 1 showed the highest selectivity against cancer cell lines compared to human fibroblasts. The most active compound against all tested cancer cell lines was 7b (half maximum effective concentration EC_{50} values were in the range from 8.2 to 24.9 μM).

SYNTHESIS OF NEW BENZOXAZOLE DERIVATIVES BEARING SULFONAMIDE MOIETY

Monika Bertašiūtė*, Birutė Grybaitė, Vytautas Mickevičius

Department of Organic Chemistry, Kaunas University of Technology, Kaunas, Lithuania
** monika.bertasiute@ktu.lt*

Benzoxazole-containing structures play a significant role in medicinal chemistry due to their broad spectrum of biological activities. As fused heterocyclic systems consisting of oxazole and benzene rings, benzoxazole derivatives have demonstrated considerable therapeutic potential, including antifungal [1], antibacterial [2], anti-inflammatory [3,4], anticancer [2], and antituberculosis [5] activities. Sulfonamides (sulfa drugs) were among the first agents to be widely and systematically used as preventive and chemotherapeutic treatments for various diseases [6]. In this context, the present study aims to synthesize novel benzoxazole derivatives bearing a sulfonamide moiety in order to develop compounds with potential biological activity.



(***I***) corresponding benzaldehyde, acetic acid, *i*-PrOH, ∆, 12 h; (***II***) 1.1 eq PIDA, ACN, ∆, 20 min; (***III***) 5 eq iodoethane, 3 eq KOH, DMF, ∆, 72 h. **a** R=H; **b** R=4-F; **c** R=2-Cl; **d** R=4-Cl; **e** R=2,6-Cl_2; **f** R=4-Br; **g** R=2-Br-5-Cl; **h** R=3-NO_2; **i** R=4-NO_2; **j** R=4-OCH_3; **k** R=3,4-$(OCH_3)_2$; **l** R=2-CF_3; **m** R=3-CF_3; **n** R=3,5-$(CF_3)_2$; **o** R=4-OCF_3; **p** R=4-SO_2CH_3; **q** R=2-OH; **r** R=3-OH; **s** R=2,4-$(OH)_2$; **t** R=2-OH-5-NO_2.

Fig. 1. Synthesis of benzoxazole derivatives bearing sulfonamide moiety

The target benzoxazole derivatives were synthesized via a two-step protocol starting from 3-amino-4-hydroxybenzensulfonamide (1). In the first step, condensation with various substituted aromatic aldehydes in 2-propanol under reflux afforded the corresponding Schiff bases 2a–t. Oxidative cyclization was first carried out using $KMnO_4$; however, the yields were low (10–29 %). Therefore, the reaction conditions were optimized by switching to (diacetoxyiodo)benzene (PIDA) in ACN, which resulted in significantly higher yields (74–95 %) of compounds 3a–p. Finally, *N*-alkylation of the sulfonamide group was performed using compound 2d and ethyl iodide in DMF under reflux to obtain 2-(4-chlorophenyl)-*N*,*N*-diethylbenzo[*d*]oxazole-5-sulfonamide (4d) (Fig. 1). The synthesized compounds were submitted evaluation of their potential biological properties.

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SYNTHESIS AND INVESTIGATION OF CYANO-SUBSTITUTED PHENOXAZINE DERIVATIVES AS RED FLUORESCENT EMITTERS

Shushanna Vardanyan[1,2]*, Simas Mačionis[1], Jūratė Simokaitienė[1], Viktorija Andrulevičienė[1], Narine Durgaryan[2], Juozas Vidas Gražulevičius[1]

[1] Department of Polymer Chemistry and Technology, Kaunas University of Technology, Kaunas, Lithuania
[2]Department of Organic Chemistry, Yerevan State University, Yerevan, Armenia Country
* *shushanna.vardanyan@ktu.edu*

Organic fluorescent compounds have attracted significant attention because of their ability to absorb light at one wavelength and emit it at a longer wavelength, with tunable emission and high quantum efficiency enabling applications across biomedicine, sensing, and optoelectronics [1]. Red-emitting materials are of growing interest because their longer wavelengths provide deeper penetration, reduce dispersion, and lower background interference, making them particularly useful for bioimaging applications. In addition, their emission characteristics are highly desirable for organic light-emitting diode (OLED) technologies, particularly in the development of full-colour and high-performance display devices [2,3]. Nevertheless, the process of creating effective red fluorescent compounds is still challenging, requiring ongoing work on molecular design and optimization.

A series of five structurally modified 10-phenyl-10H-phenoxazine derivatives are presented as potential red fluorescent materials for optoelectronic applications. The molecular design includes cyano groups and extended π-conjugation achieved through the introduction of benzene or butadiene moieties to induce red-shifted emission. The compounds were synthesized via efficient three- to four-step routes, starting from a 10-phenyl-10H-phenoxazine core prepared by Buchwald-Hartwig cross-coupling reactions. Subsequent functionalization involved bromination or formylation, followed by substitution with acrolein diethyl acetal units and final conversion of aldehyde groups to cyano groups using microwave-assisted synthesis. The thermal, electrochemical, and photophysical properties of the compounds were investigated.

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DESIGN AND SYNTHESIS OF A BODIPY-BASED NIR DYE FOR NEUTRON CAPTURE THERAPY AND RADIATION SENSING

Simona Urnikaite[1]*, Rokas Dobuzinskas[2], Mantas Grigalavicius[3], Giedre Bubniene[1], Maryte Daskeviciene[1], Vytautas Getautis[1]

[1] Department of Organic Chemistry, Kaunas University of Technology, Kaunas, Lithuania
[2] Institute of Chemical Physics, Faculty of Physics, Vilnius University, Vilnius, Lithuania
[3]Laser Research Center, Faculty of Physics, Vilnius University, Vilnius, Lithuania
* *simona.urnikaite@ktu.lt*

Neutron capture therapy (NCT) is an emerging cancer treatment modality based on the synergistic action of two relatively benign components that, when combined, generate a highly localized cytotoxic effect at the target site. The essential components of NCT include a nontoxic carrier containing a suitable nonradioactive isotope and a thermal neutron source. Among the available isotopes, boron (^{10}B) is particularly attractive due to its exceptionally high neutron capture cross-section (3838 barns; 1 barn = 10^{-24} cm^2). In addition, ^{10}B is nonradioactive, nontoxic, relatively abundant in nature (19.9%), and readily amenable to chemical functionalization [1]. In recent years, BODIPY-based theranostic agents have gained considerable attention in cancer research due to their versatile photophysical properties. According to established photochemical principles, the optical imaging and phototherapeutic performance of BODIPY dyes can be finely tuned through rational structural modification, enabling the development of multifunctional platforms [2].

Herein, we report the synthesis of a BODIPY-based near-infrared (NIR) dye (λ_{abs} = 669 nm) incorporating a boron-centered radiation-harvesting unit (Fig. 1.).

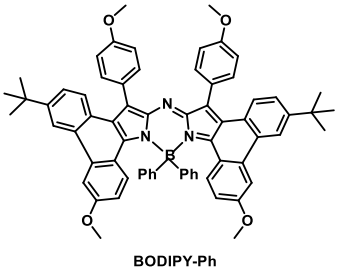

Fig. 1. Molecular structure of NIR dye BODIPY-Ph

The target derivative BODIPY-Ph was successfully synthesized in 45% yield. It will be further integrated into advanced sensor platforms for real-time, multimodal detection of ionizing radiation (neutrons, protons, and X-rays), offering high sensitivity and spatial resolution.

Acknowledgements. This work was supported by the Research Council of Lithuania (agreement No. S-MIP-25-20).

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ENVIRONMENTALLY RELEVANT EFFECTS OF PHOTOLUMINESCENT GOLD NANOCLUSTERS:LINKING NANOMATERIAL PROPERTIES TO AQUATIC BIORESPONSES

Agne Mikalauskaite[1]*, Živile Jurgelene[2], Danguole Montvydiene[2], Simonas Ramanavicius[1]

[1]State Research Institute Centre for Physical Sciences and Technology, Vilnius, Lithuania,
[2] Nature Research Centre, Institute of Ecology, Vilnius, Lithuania,
* *agne.mikalauskaite@ftmc.lt*

Photoluminescent gold nanoclusters (AuNCs), composed of a few to tens of gold atoms, are quantum-sized nanomaterials with long-lived excited states, size-dependent electronic structure, and high stability (Fig. 1a). Their growing use in biomedical and environmental fields emphasizes the need for studies linking physicochemical traits to biological effects under realistic conditions. A strong red photoluminescence at 680–700 nm with a 1.4 µs lifetime was maintained for weeks in aqueous and buffered media, showing effective suppression of fluorescence quenching. Incorporating AuNCs also improved saturation magnetization and raised the blocking temperature, indicating combined optical–magnetic properties.

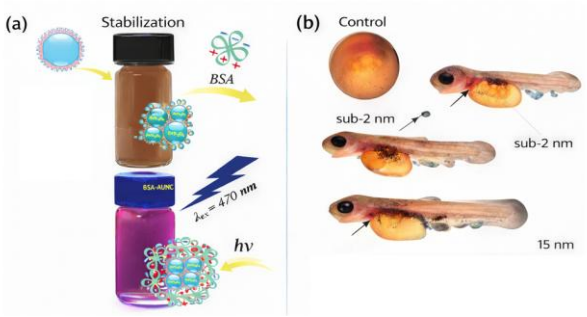

Fig. 1. Synthesis route, physicochemical properties, and biological interaction of hybrid gold nanocluster–based nanostructures: AuNC photoluminescence (a), biological uptake (b)

To evaluate biological relevance, the effects of AuNCs were investigated using aquatic primary producers and consumers as model organisms (Fig. 1b). The freshwater green alga *Desmodesmus communis* and the cladoceran *Daphnia magna* were exposed to varying concentrations of AuNCs in standard laboratory media and in natural river water. In *D. communis*, AuNCs induced time- and concentration-dependent alterations in growth dynamics, colony structure, and photosynthetic pigment composition. After 96 h exposure, changes in chlorophyll and carotenoid content, accompanied by increased malondialdehyde levels, indicated oxidative stress and membrane lipid peroxidation, with stronger effects observed in natural water matrices. In *D. magna*, AuNC exposure resulted in significant sub-lethal physiological and behavioral responses, including altered heart rate, swimming velocity, and total movement distance after 24–48 h. Behavioral endpoints proved more sensitive than acute toxicity, revealing early neurophysiological stress responses. Overall, the combined physicochemical characterization and multi-species biological assessment demonstrate that the behavior and effects of AuNCs are governed by their quantum-scale structure, surface chemistry, and environmental context. These findings underscore the importance of integrating advanced nanomaterial characterization with environmentally relevant bioassays to enable realistic risk assessment and the safe-by-design development of photoluminescent nanomaterials.

NOVEL PYRAZOLE RING-CONTAINING FLAVONE AND ISOFLAVONE ANALOGUES: SYNTHESIS AND CHARACTERISATION

Melita Petrikė[1]*, Eglė Arbačiauskienė[1], Algirdas Šačkus[2]

[1] Department of Organic Chemistry, Kaunas University of Technology, Kaunas, Lithuania
[2] Institute of Synthetic Chemistry, Kaunas University of Technology, Kaunas, Lithuania
** melita.petrike@ktu.lt*

Flavones can be found naturally in various plant parts, such as leaves, fruits, and flowers, while isoflavones are mainly found in leguminous plants [1]. They both exhibit diverse biological activities, for example, anticancer, antioxidant, anti-inflammatory [2,3], and antibacterial [2,4] activity. The aim of this work was to synthesize pyrano[2,3-*c*]pyrazol-4(2*H*)-ones containing flavone and isoflavone analogues. Pyrazole derivatives exhibit a variety of biological properties, including analgesic, anti-inflammatory, antibacterial, antimalarial, antifungal, antioxidant, and anticancer effects [5]. Consequently, the synthesis of pyrazole ring-containing (iso)flavone analogues might lead to novel structures with beneficial biological activities.

In a two-step synthesis approach, 1-phenyl-1*H*-pyrazol-3-one was converted to 1-(3-hydroxy-1-phenyl-1*H*-pyrazol-4-yl)ethan-1-one. The obtained compound was further treated with various aldehydes in basic conditions and iodine, which resulted in the formation of 6-arylpyrano[2,3-*c*]pyrazol-4(2*H*)-ones. Similar reaction of 1-(3-hydroxy-1-phenyl-1*H*-pyrazol-4-yl)ethan-1-one with various aldehydes in basic conditions and H_2O_2 resulted in the formation of another group of target products – 6-aryl-5-hydroxypyrano[2,3-*c*]pyrazol-4(2*H*)-ones [6]. The hydroxy group of the obtained product was converted to a triflate, followed by palladium-catalyzed methoxycarbonylation reaction. Obtained methyl esters were further functionalized by forming carboxylic acids and amides. For the expansion of the study, 1-(3-hydroxy-1-phenyl-1*H*-pyrazol-4-yl)ethan-1-one was used in a step-wise synthetic approach for the formation of 5-iodopyrano[2,3-*c*]pyrazol-4(2*H*)-one, which was converted to targeted 5-arylpyrano[2,3-*c*]pyrazol-4(2*H*)-ones via Suzuki-Miyaura coupling reaction. The structures of synthesized compounds were confirmed by ^{1}H, ^{13}C, and ^{15}N-NMR spectroscopy.

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CONTINUOUS MULTIZONAL POLY(ε-CAPROLACTONE) BASED OSTEOCHONDRAL SCAFFOLD INCORPORATING FUNCTIONALIZED HYDROGELS FOR *IN VITRO* MODELLING

Aiste Pupiute[1]*, Darius Ciuzas[1], Odeta Baniukaitiene[1], Dainius Martuzevicius[1], Edvardas Bagdonas[2], Eiva Bernotiene[2], Tomas Ragauskas[2], and Edvinas Krugly[1]

[1] Faculty of Chemical Technology, Kaunas University of Technology, Kaunas, Lithuania
[2] State Research Institute Centre for Innovative Medicine, Vilnius, Lithuania
* *aiste.pupiute@ktu.lt*

Osteochondral tissue exhibits a complex zonal architecture and limited intrinsic healing capacity, yet the development of *in vitro* models that reproduce its structural organization and interfacial features remains challenging [1-2]. This study aimed to develop a multizonal osteochondral *in vitro* model by integrating a zone specific scaffold with methacrylated hyaluronic acid (MeHA) hydrogel functionalized with chondroitin sulfate (CS) and hydroxyapatite particles (HAp).

A multizonal PCL scaffold was fabricated using melt electrospinning, solution electrospinning and solution blow spinning. Scaffolds were treated with non-thermal plasma (NTP) to enhance hydrophilicity, then characterized for mechanical and physicochemical properties. MeHA was synthesized and characterized by ^{1}H NMR and FT-IR. Hydrogel formulations with different MeHA and LAP photoinitiator concentrations were assessed by photorheology and dynamic rheology to identify the most suitable composition. The selected hydrogel was functionalized with CS and HAp for the chondral and osseous scaffold compartments, respectively. Swelling, degradation, and compressive behavior of scaffold and hydrogel composites were evaluated.

The scaffold exhibited an interconnected porous structure. NTP treatment reduced the WCA from 108 ±1.7° to 51.3 ±1.8°. MeHA was successfully synthesized with a degree of substitution of 63%. All hydrogel formulations showed rapid photocrosslinking, with gelation times of 4–6 s. Based on rheological analysis, the 2.0% MeHA hydrogel crosslinked with 0.1% LAP was selected for further studies because its G’ value at 25 Hz (377.5 ±9.5 Pa) was similar to that of 5.0% GelMA (380.1 ±7.6 Pa). CS incorporation had little effect on viscoelastic behavior, whereas HAp markedly increased hydrogel stiffness. MeHA-CS and MeHA-HAp hydrogels showed lower swelling and slower degradation than unfunctionalized MeHA. Incorporation of MeHA hydrogel into the multizonal scaffold increased the apparent compressive modulus from 100 ±30 to 193 ±16 kPa, while maintaining good recovery after cyclic compression.

The developed multizonal scaffold and functionalized hydrogel system successfully reproduced key structural and physicochemical features of osteochondral tissue and provided tunable mechanical properties relevant for interface modelling. This biomimetic *in vitro* model enables investigation of osteochondral interactions, disease progression, and therapeutic testing while advancing 3R principles and reducing animal use.

Acknowledgements. This study was supported by Research Council of Lithuania. Grant No. S-MIP-24-38.

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PREPARATION ANTIMONY SELENIDE FILMS ON FTO SUBSTRATE

Remigijus Ivanauskas*, Evelina Kasparavičiūtė, Skirma Žalenkienė

Department of Physical and Inorganic Chemistry, Kaunas University of Technology, Kaunas, Lithuanian,
** remigijus.ivanauskas@ktu.lt*

The depletion of fossil fuel reserves and the resulting energy shortages have become critical issues for socio-economic development and potential drivers of global crises. Therefore, the development of reliable and sustainable renewable energy sources is essential to mitigate these problems. Among the available alternatives, photovoltaic technologies are considered one of the most promising solutions to address the global energy shortage. In recent years, composite thin-film solar cells have attracted considerable research interest due to their low material consumption and reduced energy costs during their fabrication. Currently, the most widely developed composite thin-film solar cell technologies include cadmium telluride (CdTe), copper indium gallium selenide (CIGS), and copper zinc tin selenide (CZTS), which have achieved energy conversion efficiencies of 22.1%, 23.35%, and 12.6%, respectively [1, 2]. Antimony selenide (Sb_2Se_3), a member of the thin-film photovoltaic material family, has attracted considerable scientific interest in recent years as a promising functional material for photovoltaic and optoelectronic applications. Sb_2Se_3 possesses a near-optimal optical band gap of approximately 1.2 eV, a high absorption coefficient exceeding 10^5 cm^{-1}, moderate charge-carrier mobility (~10 cm^2 V^{-1} s^{-1}), a relatively long carrier lifetime (~60 ns), and low material cost. In addition, Sb_2Se_3 is considered environmentally benign compared with many other compound semiconductors and is composed of earth-abundant elements, making it a strong candidate for the development of next-generation clean and sustainable solar energy technologies. Based on these data, the main objective of this study was to synthesize Sb_2Se_3 thin films on FTO substrates using different preparation methods and to investigate how the synthesis route influences their phase composition, crystallinity, morphology, and optical properties. The Sb_2Se_3 thin films were characterized by X-ray diffraction (XRD) to analyze their crystal structure, scanning electron microscopy (SEM) and atomic force microscopy (AFM) to examine surface morphology, and energy-dispersive X-ray spectroscopy (EDS) to determine elemental composition. The optical properties of the films were evaluated using UV–visible spectroscopy.

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METHYLENE BULE AND AZURE A ADSORPTION ON TITANIUM CARBIDE MXENES: A FIRST-PRINCIPLES AND EXPERIMENTAL STUDY

Enayat Mohsenzadeh [1]*, Aswathi Raveendran[1], Germante Paulikaite[1], Martynas Talaikis[1], Arnas Naujokaitis[1], Agne Mikalauskaite[1], Oleksiy Gogotsi[2], Simonas Ramanavicius[1]

[1] Center for Physical Sciences and Technology, Vilnius
[2] Carbon-Ukraine (Y-Carbon LLC), Kyiv, Ukraine
* *enayat.mohsenzadeh@ftmc.lt*

Titanium carbide MXenes are two-dimensional materials derived from MAX phases, featuring surface terminations (–F, –O, –OH) that provide abundant active sites and enable strong interactions with a wide range of adsorbates. Owing to their high surface area, metallic conductivity, and tunable surface chemistry, MXenes have demonstrated excellent adsorption performance toward organic dyes and heavy metal ions, making them highly promising for water purification applications [1,2].

$Ti_3C_2T_x$ (T_x denotes terminating functional group) MXenes are typically synthesized via selective etching of Al element from Ti_3AlC_2, resulting in multilayered structures. In our study, the successful formation of MXene was confirmed by XRD and Raman spectroscopy. SEM analysis revealed a stacked, sheet-like morphology of MXenes. A comparative adsorption study was conducted using methylene blue and azure A, two organic dyes with methylene blue having additional methyl group, to elucidate the adsorption mechanism. The experimental results indicate a higher adsorption affinity of MXenes toward methylene blue compared to azure A, attributed to differences in their functional groups. The influence of pH on adsorption behavior was also evaluated, revealing enhanced adsorption of methylene blue over azure A within the pH range of 3–6. Additionally, MXenes demonstrated good reusability, maintaining effective adsorption performance.

The adsorption mechanism was further elucidated by density functional theory (DFT) calculations. Density of states (DOS) analysis revealed that interactions between MXene surfaces and dye molecules induce shifts in the Fermi level, depending on surface termination. –OH terminated MXenes exhibited the strongest adsorption energies, attributed to enhanced electrostatic interactions and hydrogen bonding, compared to −O and −F terminations. Charge transfer analysis showed that for −O and −F terminations, electrons transfer from the dye to the MXene, whereas the opposite occurs for –OH surfaces. These interactions lead to distinct Fermi level realignments and confirm termination-dependent electronic modulation of adsorption behavior and higher adsorption for methylene blue.

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ELECTROCHEMICAL BEHAVIOR OF AISI GRADE STEELS IN NITRATE REDUCTION REACTION

Eugenijus Valatka*, Simonas Vaitkevičius

Department of Physical and Inorganic Chemistry, Kaunas University of Technology, Lithuania,
* *eugenijus.valatka@ktu.lt*

The growing need for ammonia and inevitable transition towards Net Zero puts increasingly more pressure on current natural gas-based ammonia production methods and forces to look for greener solutions. Electrochemical ammonia production could reduce the reliance on fossil fuels and enables to achieve near zero emission ammonia production [1]. This process efficiency is limited by competing hydrogen evolution reaction (HER), thus the search for more efficient and selective catalysts for electrochemical nitrogen reduction reaction (eNRR) is one of the main fields for improvement in making this process viable alternative to Haber-Bosch process [2].

The catalysts based on iron have been used in production of ammonia for more than a century. Due to their abundance, low price and high catalytic activity, Fe-based materials are extensively used in majority of catalysts. The activity is further improved by the use of catalyst promoting additives [3].

The aim of this work was to study the activity of AISI grade steels in electrochemical nitrate reduction reaction (NRR).

Electrochemical activity of AISI grade steels were tested by reducing nitrate ions in 0.1 M KNO_3 and 0.1 M KNO_3 + 0.1 M K_2SO_4 aqueous solutions. Voltammetry, chronoamperometry, chronopotentiometry measurements were carried out in three-electrode cell consisting of stainless steel plate (2 cm^2) as a working electrode, Ag,AgCl|KCl_{sat} as a reference electrode and Pt wire (15 cm^2) as a counter electrode.

The experimental results showed that electrocatalytic activity of tested steels increases in this order AISI 316<AISI 321<AISI 302<AISI 304. AISI 304 steel also showed highest corrosion resistance, the corrosion rate being $1{,}41 \cdot 10^{-4}$ mm/y. The parameters of Tafel equation were calculated to provide additional information on NRR mechanism and rate-limiting processes. It has been found that sulfate ions have a positive effect on the electrochemical reduction of nitrate to ammonia, increasing the selectivity of the reaction towards ammonia.

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SILVER-DOPED CARBONATED HYDROXYAPATITE GRANULES FOR ANTIBACTERIAL BONE REGENERATION

Gabriele Meizyte*, Maab Abdulsamad Ahmed Elsheikh, Inga Grigoraviciute, Aivaras Kareiva

Institute of Chemistry, Faculty of Chemistry and Geosciences, Vilnius University, Vilnius, Lithuania
* gabriele.meizyte@chgf.vu.lt

Bone repair requires scaffolds that mimic native mineral tissue. Carbonated hydroxyapatite (CHA, $Ca_{10-a}(CO_3)_b(PO_4)_{6-c}(OH)_{2-d}$) meets this need as the principal inorganic component of bone and is widely used as a graft material. It is more biocompatible than another common artificial bone substitute hydroxyapatite (HA, $Ca_{10}(PO_4)_6(OH)_2$) but less thermally stable. Overall, CHA offers a more suitable balance of biocompatibility and stability than HA for bone repair [1,2.] Such unmodified materials, however, lack intrinsic antimicrobial activity, leaving implants vulnerable to infection. Silver ions were shown to possess antibacterial effects and were successfully incorporated into CHA [3].

The CHA granules (150–500 µm) were synthesized via a low-temperature dissolution–precipitation method using naturally abundant calcium sulfate (gypsum). The reaction was conducted in aqueous media without organic reagents, aligning with environmentally friendly synthesis principles. Silver was incorporated relative to the initial CHA granule mass at 0.5, 1.0, 2.5, 5.0, and 7.5 wt% to systematically study its antibacterial effect. The characterization of CHA granules focused on structural, chemical, and morphological analysis via X-raydiffraction, Fourier transform infrared and Raman spectroscopies, scanning electron microscopy, and surface area measurements.

The study's outcome is to functionalize the CHA bioceramics by embedding silver into the CHA granules, and in this way produce an advanced antibacterial biomaterial suitable for bone regeneration.

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