

9th Meeting on CHEMISTRY & LIFE for Sustainable Future

# **BOOK OF ABSTRACTS**

# **OP1: Bio-organic Semiconductors for a Sustainable Electronics and Their Bio-medical Integration**

## Niyazi Serdar Sariciftci<sup>1</sup>

<sup>1</sup> Linz Institute for Organic Solar Cells (LIOS) and Institute of Physical Chemistry at the Johannes Kepler University of Linz, Austria, www.lios.at, Email: Serdar.Sariciftci@jku.at.

## Keywords: Bioelectronics, bio-organic semiconductors, biomedical optoelectronic implants

Bio-organic electronics is emerging rapidly in the scientific world. Organic semiconductors have already been established in organic light emitting diodes (OLED) and organic photovoltaics (OPV) as well as organic field effect transistors (OFET).



Figure 1: Illustration of interface between life-biosciences and electronic world.

Generally, bioelectronics has been a dream of cybernetics for quite some time. The pioneering work of Peter Fromherz (Max Planck Institute for Biochemistry) interfacing the neurons with silicon circuits go back several decades. Since then, however, the bioelectronics has been limited to silicon based electronic circuits for quite some time.

Recently, bio-compatible, bio-inspired and/or bioorigin organic semiconductors have opened up a new avenue to realize this dream of interfacing biology/medicine with electronic circuits. Organic semiconductors, especially bio-organic, bio-compatible semiconductors display a list of properties which are important for the interfacing of biological systems with electronic world: Their biocompatibility, non-toxicity, processability and operational stability in aqueous media are often much better than the silicon-based circuits.

To make an interface with any biosystems, the transformation of the electrical information into ionic and protonic information is necessary. Biosystems are often based on ionic transport and signal transduction based on electrochemical principles as opposed to electronic world which use normally the electronic conduction based on solid state physics. In such a transformation of the signal from electronic world to the biological world, we need materials and systems as "transducers", which can sustain electronic as well as ionic conduction and their translation into each other. Organic semiconductors can offer this possibility. Therefore, we suggest that the future of cybernetics might be using more and more organic/bioorganic semiconductors.

On the other hand, the green Electronics itself is also important to sustain a sound and healthy environment. We have already a problem with our electronic waste in the world today. Humanity is not able to create a sustainable cycle for production, use and end-of-life of our electronic gadgets and instruments. Often such highly valuable products are landing in ordinary garbage dumps, polluting the environment, wasting valuable and precious materials as well.

Akio Morita, the chairman of SONY Incorporation has once stated: "We are moving from consumer electronics to consumable electronics".

Thus, the use of organic and bio-degradable, biocompatible materials is quite advantageous for these many different applications.

## References

- [1] M. Irimia-Vladu, E. D. Glowacki, N. S. Sariciftci, S. Bauer (Eds.) *Green Materials for Electronics*, Wiley VCH, Weinheim, 2018, p. 352.
- [2] R. Shinar, J. Shinar, Organic Electronics in Sensors and Biotechnology, McGraw Hill, 2009, p. 448.
- [3] M. Irimia-Vladu, N. S. Sariciftci, S. Bauer, J. Mater. Chem. 21 (2011) 1350-1361.

# OP2: From Trash to Treasure – Importance of Microbes in Circular Economy

**Radecka Iza**<sup>1</sup>, Tchuenbou-Magaia Fideline<sup>1</sup>, Parati Mattia<sup>1</sup>, Mansoor Zinnia<sup>1</sup>, Gupta Abhishek<sup>1</sup>, Johnston Brian<sup>1</sup>, Khalil Ibrahim<sup>1</sup>, Mendrek Barbara<sup>2</sup>, Adamus Grazyna<sup>2</sup>, Kowalczuk Marek<sup>2</sup>

- <sup>1</sup> University of Wolverhampton, Faculty of Science & Engineering, Wulfruna Street, Wolverhampton, WV1 1LY, United Kingdom, Email: I.Radecka@wlv.ac.uk.
- <sup>2</sup> Centre of Polymer and Carbon Materials, Polish Academy of Sciences, M. Curie-Sklodowskiej 34, 41-819 Zabrze, Poland

Keywords: wastes, PHA, bacterial cellulose, poly-gamma glutamic acid, biomaterials.

Microorganisms are key to a functioning circular economy, where natural resources, including biological waste, is converted by microbial cells into added value products (e.g. biogas, bioethanol, biodegradable polymers, compost) utilized by society. Microbial polymers have an enormous potential as they can be produced from renewable biogenic resources (waste) under well controlled conditions. This approach can help address growing concerns about the depletion of natural resources caused by an increasing human population, waste production, and accumulation.

Over the past few decades many biopolymers originating from various types of microorganisms have

been reported. This presentation will discuss an integrated biotechnological/chemical process, which allows the transformation of agricultural and other biorefinery byproducts into value-added biodegradable polymeric materials which may be used in the areas of agriculture, cosmetics, medicine, as well as in household products, coating systems and as additives to compostable plastic packages of extended shelf life.

This presentation will also describe the biosynthesis and production of biodegradable microbial polymers and their most important industrial applications and ecological advantages.

## **OP3: Designing Organic Semiconducting Polymers for Transistors**

## McCulloch lain<sup>1</sup>

<sup>1</sup> Andlinger Center for Energy and the Environment and Department of Electrical and Computer Engineering, Princeton University, Princeton, NJ, 08544, USA, Email: iain.mcculloch@chem.ox.ac.uk

## Keywords: polymer, organic electronics, semiconductor

This presentation will discuss current understanding of the molecular design features responsible for optimising charge transport in organic semiconducting polymers. Organic semiconducting polymers have been shown to be promising candidates to enable high charge carrier mobility in organic thin film transistors, which can find use in flexible displays and other electronic applications. We will take a close look at the molecular features responsible for the high charge carrier mobility of the indacenodithiophene-co-benzothiadiazole copolymer1-5 a benchmark semiconducting polymer employed in organic transistors. This will involve highlighting the influence of conformational coplanarity and side-chain assisted self-assembly to create efficient one-dimensional transport along conjugated polymer backbones, with sterically free "crossing points" allowing interchain hopping. Understanding the impact of both the organic semiconducting polymer design and processing conditions, on both molecular conformation and thin film microstructure has been demonstrated to be essential in achieving the optimal transport properties.

## References

- W. Zhang, J. Smith, S.E. Watkins, R. Gysel, M. McGehee, A. Salleo, J. Kirkpatrick, S. Ashraf, T. Anthopoulos, M. Heeney, I. McCulloch, J. Am. Chem. Soc. 132 (2010) 11437-11439.
- X. Zhang, H. Bronstein, A.J. Kronemeijer, J. Smith, Y. Kim, R.J. Kline, L.J. Richter, T.D. Anthopoulos, H. Sirringhaus, K. Song, M. Heeney, W. Zhang, I. McCulloch, D.M. DeLongchamp, *Nat. Commun.* 4 (2013) 3238/1-3238/9.
- [3] D. Venkateshvaran, M. Nikolka, A. Sadhanala, M. Zelazny, A.J. Kronemeijer, V. Pecunia, I. Nasrallah, I. Romanov, K. Broch, H. Sirringhaus, V. Lemaur, Y. Olivier, J. Cornil, D. Beljonne, M. Kepa, M. Hurhangee, I. McCulloch, D. Emin, *Nature* 215 (2014) 384-8.
- [4] A. Wadsworth, H. Chen, K.J. Thorley, C. Cendra, M. Nikolka, H. Bristow, M. Moser, A. Salleo, T.D. Anthopoulos, H. Sirringhaus, I. McCulloch, *J. Am. Chem. Soc.* 142 (2020) 652-664.
- [5] C. Cendra, L. Balhorn, W. Zhang, K. O'Hara, K. Bruening, C.J. Tassone, H.G. Steinrück, M. Liang, M.F. Toney, I. McCulloch, M. L. Chabinyc, A. Salleo, C.J. Takacs, *ACS Macro Letters* 10 (2021) 1306-1314.

## OP4: CO<sub>2</sub> Mineralization: CCU for and by building materials

## Skocek Jan<sup>1</sup>, Pato Nicolas<sup>1</sup>, Zajac Maciej<sup>1</sup>

<sup>1</sup> Heidelberg Materials AG, Global R&D, Oberklamweg 2-4, Leimen 69181, Germany, Email: jan.skocek@heidelbergmaterials.com

## Keywords: CO<sub>2</sub> mineralization, Concrete, Carbonation, Sustainability, Recycling

Concrete is the most widely used construction material in the world, and it is composed of cement, water, sand, and aggregates. Cement production is one of the major sources of global  $CO_2$  emissions, accounting for about 8% of the total anthropogenic emissions. Most of the  $CO_2$ emissions come from the calcination of limestone, which is a hard-to-abate process that can only be decarbonized by applying Carbon Capture and Storage (CCS) technologies. The overall volume of CCS applied can be lowered by reducing the content of clinker in cement and of cement in concrete via the use of supplementary cementitious materials with lower environmental impacts.

Concrete has a long service life and can be fully recycled at the end of its life cycle. However, the circular potential of concrete is largely untapped, as most of the demolished concrete is used for low-grade applications such as road-base or backfill, while only a small fraction is reused as aggregate for new concrete. For concrete, most aggregates are extracted virgin materials, such as sand and gravel, which are becoming scarce and expensive resources.

 $CO_2$  mineralization has the potential to address both aforementioned issues at once – improve concrete circularity and lower the overall CO2 emissions associated with its production. It can be efficiently applied at three stages of the concrete value chain [1]:

- to valorize byproducts and waste materials from other industries via a carbonationinduced activation converting these into reactive supplementary cementitious materials (SCMs),
- to harden fresh concrete product via earlyage carbonation of cements and alternative binders which includes non-hydraulic binders,
- to carbonate recycled concrete aggregates or fines to bind carbon and enhance properties of these materials.

The last option is especially attractive as it is independent of material flows from other industries, and it also facilitates circular reuse of sand and aggregates. ReConcrete is a dedicated technology combining a novel

## References

- [1] M. Zajac et al., Energies 15 (2022), 3597.
- [2] J. Skocek et. al, Scientific Reports 10 (2020) 5614.
- [3] M. Zajac, J. Skocek. L. Golek, J. Deja, Journal of Cleaner Production 387 (2023) 135743.

concrete recycling process with the  $CO_2$  mineralization applied as a CCS technology for cement production or other  $CO_2$ -emitting industrial processes. The technology is illustrated in Figure 1.



Figure 1: ReConcrete technology for complete recycling of concrete including old cement and process CO<sub>2</sub>emissions

First, the selective separation of demolished concrete into clean aggregates and sand plus fine fraction concentrating the hydrated cement (Recycled Concrete Paste, RCP) takes place. The recycled aggregates and sand can fully substitute virgin materials in fresh concrete production as the adhered cement paste has been removed. The RCP, due to its fineness and composition, can selectively and rapidly bind CO<sub>2</sub> from a raw flue gas and hence offers an alternative low energy and low-cost CCS technology [2]. The carbonated RCP becomes a highly reactive pozzolanic material suitable for clinker replacement in composite cements [3].

With the ReConcrete technology, old concrete can be fully recycled into new concrete and cement, including the process emissions from limestone decomposition during clinker production. It is hence a vital contribution to address both the decarbonization and circularity ambitions of concrete industry.

The talk will introduce all three aforementioned CO2mineralization pathways in detail, ranging from basic research to first experience at commercially relevant scale.

# **OP5: Catanionic Systems for a Sustainable Future: Applications as Drug Carriers**

## Lin Jia-Rong<sup>1</sup>, Chang Chien-Hsiang<sup>1</sup>

<sup>1</sup> Department of Chemical Engineering, National Cheng Kung University, No. 1 University Road, Tainan 701, TAIWAN, Email: changch@mail.ncku.edu.tw

Keywords: catanionic vesicle, drug delivery system, ion pair amphiphile, mixed cationic/anionic surfactants, vesicular structure

An approach to destroy the stable structures of surfactant aggregates in aqueous phase is to form mixed cationic/anionic surfactant mixtures, or ion pair amphiphiles. In this study, a high value application of ion pair amphiphiles as raw materials for drug delivery carriers was demonstrated. Ion pair amphiphiles with various double-chained and triple-chained structures were prepared from mixed surfactant systems, and catanionic vesicles were then fabricated from the ion pair amphiphiles by applying a forced formation process. For ion pair amphiphiles with double-chained structures, charge character and physical stability of the catanionic vesicles could be controlled by adopting additives of charged double-chained surfactants and cholesterol. The roles of added cholesterol in the enhanced physical stability of the catanionic vesicles were probably attributed to its ability to modulate bilayer fluidity of the catanionic vesicles. For triple-chained ion pair amphiphiles, stable catanionic vesicles were successfully fabricated without the addition of charged surfactants or cholesterol (Figure 1), and charged character of the catanionic vesicles could be controlled by the preferential dissociation of the cationic or anionic moiety of the ion pair amphiphiles. Bilayer fluidity of the catanionic vesicles could also be modulated by the addition of cholesterol, and thus the phase transition temperatures of the vesicular structures were possible to be adjusted for specific applications. For catanionic vesicles fabricated from double-chained and triple-chained ion pair amphiphiles, encapsulation behavior for hydrophilic and hydrophobic materials were examined, and the results suggested that ion pair amphiphiles could be used as raw materials for fabricating catanionic vesicles with potential of being applied as drug delivery carriers.



*Figure 1: Stable catanionic vesicles could be fabricated from a triple-chained ion pair amphiphile without additives.* 



Figure 2: Bilayer fluidity of the catanionic vesicles fabricated from a triple-chained ion pair amphiphile could be modulated by the addition of cholesterol.

## Acknowledgement

This work was supported by the National Science and Technology Council of Taiwan.

# OWK: Sustainable Process Development on Biorefinery Electrification and Chemical Recycling of Post-Consumer Bioplastics

## Koutinas Apostolis<sup>1</sup>

<sup>1</sup> Agricultural University of Athens, Department of Food Science and Human Nutrition, Iera Odos 75, 11885, Athens, Greece, Email: akoutinas@aua.gr

## Keywords: Biorefinery electrification, circular economy, biopolymers, bioprocess

Restructuring conventional biorefineries and bioprocesses using crude renewable resources for the production of bio-based chemicals and polymers is essential in order to boost the transition to the circular economy era. This study presents the restructuring of conventional biorefineries and bioprocesses through the implementation of nonthermal plasma for pretreatment of lignocellulosic biomass, electrochemical membrane extraction of carboxylic acids during fermentation and chemical recycling of post-consumer bioplastics as novel and sustainable processes. The replacement of steam and chemicals by renewable electricity could reduce the environmental impact of conventional bioprocesses and biorefineries. Furthermore, the utilisation of renewable electricity could lead to higher polysaccharide to sugar as well as sugar to metabolic products conversion yields. The chemical recycling of post-consumer bioplastics could generate carbon sources for fermentation processes leading to circular reproduction of biopolymers minimizing virgin feedstock requirements and improving resource efficiency. The methodological approach will focus on replacing specific unit operations in conventional bioprocesses and biorefineries or using degradation products from post-consumer bioplastics as carbon sources in fermentation processes for the circular production of biopolymers. Specific case studies will be presented to demonstrate the sustainability potential of the proposed concepts. For instance, production using non-thermal plasma PHB pretreated food industry side streams (e.g. brewers' spent grains), recirculation of post-consumer PHBbased packaging for the production of new PHB via fermentation and simultaneous production and extraction of succinic acid using a novel electrochemical membrane bioreactor will be presented as case studies.

# OW1: Thermophiles: A Promising Platform for Advancing Sustainable Industrial Microbial Biotechnology

**Obruča Stanislav**<sup>1</sup>, Pernicová Iva<sup>1</sup>, Kouřilová Xenie<sup>1</sup>, Sedlář Karel<sup>2</sup>, Dvořák Pavel<sup>3</sup>, Řeháková Veronika<sup>1</sup>, Sedláček Petr<sup>1</sup>, Šlosárová Katarina<sup>1</sup>, Musilová Jana<sup>2</sup>, Hrabalová Vendula<sup>1</sup>, Heřmánková Kristýna<sup>2</sup>, Ieremenko Anastasiia<sup>3</sup>, Šafránek David<sup>4</sup>

- <sup>1</sup> Faculty of Chemistry, Brno University of Technology, Purkyňova 118; 612 00 Brno, Czech Republic, Email: obruca@fch.vut.cz
- Faculty of Electrical Engineering and Communication, Brno University of Technology, Technicka 12, 612 00 Brno, Czech Republic
- <sup>3</sup> Faculty of Science, Masaryk University, Kamenice 753/5, 625 00 Brno, Czech Republic
- <sup>4</sup> Faculty of Informatics, Masaryk University, Botanická 68a, 602 00 Brno, Czech Republic

Keywords: polyhydroxyalkanoates; thermophiles; *Caldimonas thermodepolymerans; Aneurinibacillus* spp.

Polyhydroxyalkanoates (PHA) are biodegradable, biocompatible, and bio-based polyesters synthesized by various prokaryotes, offering a sustainable alternative to synthetic petrochemical polymers. However, the high production costs associated with PHA limit their competitiveness with conventional synthetic polymers. Employing extremophiles as hosts for PHA biosynthesis presents significant advantages, primarily due to their natural resistance to contamination by ubiquitous microflora. This resistance enables production processes that can operate in semi-sterile or non-sterile conditions, even under continuous or semi-continuous modes, thereby substantially reducing costs. Our research has focused on the exploration and screening of thermophiles capable of PHA biosynthesis. Compared to halophiles, the potential of thermophiles for PHA production remains largely unexplored, with only a few thermophilic strains reported to possess this capability. To address this gap, we systematically screened a selection of thermophilic strains from public microbial collections, aiming to identify novel and potent PHA producers. Among the promising candidates identified are Tepidimonas taiwanensis and Caldimonas thermodepolymerans, both of which show strong potential for PHA production from various waste resources. In addition to strain selection, we developed a novel isolation protocol that facilitates the identification of PHA-accumulating thermophiles from complex microbial consortia such as compost and activated sludge. This approach led to the discovery of several promising thermophiles, including isolates from the genus Aneurinibacillus, which exhibit a unique ability to incorporate diverse monomer units into the PHA polymer chain. Currently, we are leveraging bioinformatics and systems biology tools to develop metabolic models for these thermophiles, particularly Caldimonas thermodepolymerans. Using metabolic engineering, we aim to optimize these microorganisms as robust biotechnological platforms not only for the production of PHA but also for other valuable bioproducts. This research highlights the untapped potential of thermophiles in the sustainable production of biopolymers and sets the stage for future industrial applications.

## Acknowledgement

This study was supported by grant project GACR GA22-10845S.

# OW2: Bacterial Cellulose Hydrogel: An Emerging Biomaterial for Chemistry and Life

## Saha Nabanita<sup>1</sup>

<sup>1</sup> Centre of Polymer Systems, University Institute, Tomas Bata University in Zlin, Trida Tomase Bati 5678, 76001 Zlin, Czech Republic, Email: nabanita@utb.cz

## Keywords: Bacterial Cellulose, Biomaterial, Emerging material, Bacterial Cellulosed Hydrogel

In current eras, with the development of green chemistry and nanotechnology, bacterial cellulose (BC) has received increased attention not only in academia, and industry but also in day- to- day life especially in the field of healthcare. BC hydrogel is considered a natural hydrogel that inherits the advantages of green chemistry and little toxicity [1]. Besides this, such high-strength fibers of BC provide stronger mechanical properties for materials, making up for the limitations of traditional natural hydrogels such as low strength and poor toughness etc. Pure natural BC hydrogel fiber has good bio-ion conductivity and light-guiding performance, making it a great application prospect for preparing various emerging materials: in the field of sensors, food packaging, medical devices, wound dressing material, leather substitute materia, I and so on [2-4]



Figure 1: Visual Image about Production of Bacterial Cellulose/Bacterial Cellulose Hydrogel at CPS, TBU in Zlin.

## References

- [1] X. Pan, J. Li, N. Ma et.al., Chemical Engineering Journal, 461 (2023) 142062.
- [2] J. Wang, J. Tavakolib, Y. Tang, Carbohydrate Polymers, 219 (2019) 63-76.
- [3] H.T. Nguyen, N. Saha et.al., *Cellulose*, 28 (2021), 9335-9353.

[4] P. Basu, N. Saha, P. Saha, International Journal of Polymeric Materials and Polymeric Biomaterials, 68 (2019) 134-144.

## Acknowledgement

This work is partially supported by Twinning for Development of World-Class Next Generation Batteries (Twin VECTOR) project Number: 101078935 from December 2022, and is acknowledged with pleasure.

BC is a nano-sized cellulose fibers produced by bacteria that is terminated with abundant hydroxyl groups. The BC producing bacteria are mainly Gram – negative bacteria. The most well-known bacteria is *Komagataeibacter* (formerly named as *Gluconacetobacter xylinus*, a Gram-negative obligate aerobic bacterium that efficiently metabolizes multiple carbon and nitrogen sources to generate BC. The bio-synthesis of BC involves the participation of multiple enzymes and reactions at multiple stages, which can be summarized as **four** steps:

(1) **Glucose** is converted to glucose–6–phosphate by *phosphorylation of glucokinase*;

(2) **Glc–6–P** is converted to glucose–1–phosphate by isomerization *of gluconophosphate mutase*;

(3) **Glc–1–P** is converted to uridine diphosphate glucose by *UDP–glucose pyrophosphorylase*;

(4) **UDP-glucose** polymerized into linear  $\beta$ -(1-4)-glucan chain by *Cellulose synthase* to form **Bacterial Cellulose** [1].

BC is basically a linear polysaccharide composed of thousands of repeating D–glucose connected by  $\beta$ –1, 4–glycosidic bonds. BC possesses a high aspect ratio and a large specific surface area with a diameter in the 10–100 nm range and length reaching several microns.

In this platform, I propose to discuss about a comprehensive review on recent advances of biosynthesis of BC hydrogel and its application including our research achievement on 'Bacterial Cellulose Hydrogel'.

# OW3: An Initial Genome Editing Toolset for Caldimonas Thermodepolymerans

leremenko Anastasiia<sup>1</sup>, Lipovská Kristýna<sup>1</sup>, Kouřilová Xenie<sup>2</sup>, Obruča Stanislav<sup>2</sup>, Dvořák Pavel<sup>1</sup>

- <sup>1</sup> Masaryk University, Dpt. of Experimental Biology, Section of Microbiology, Kamenice 5/E25, 62500 Brno, Email: ieremenko@sci.muni.cz, Email: pdvorak@sci.muni.cz
- <sup>2</sup> Brno University of Technology, Institute of Food Science and Biotechnology, Purkyňova 464/118, 61200, Brno

## Keywords: thermophilic bacterium, genome editing, PHA producer

Caldimonas thermodepolymerans DSM 15344, a moderately thermophilic Gram-negative bacterium, is an attractive microbial candidate for the Next-Generation Industrial Biotechnology due to its ability to utilize sugars from plant biomass and convert them efficiently to poly(3hydroxybutyrate). Unlike the majority of polyhydroxyalkanoate producers, *C. thermodepolymerans* prefers xylose over glucose [1]. Production potential of this promising thermophilic bacterium could be further enhanced by genetic and metabolic engineering but suitable engineering tools are not yet available.

This study describes the development of genetic engineering tools for *C. thermodepolymerans*. The work includes the optimization of transformation protocol, selection of suitable antibiotics and antibiotic resistance

genes, development and adoption of plasmid-based tools for genome editing (gene insertion and deletion), and search for reliable regulatory sequences. Within this project, we created two genome editing systems utilizing gfp and sacB genes for mutant selection. Additionally, we demonstrated the significant impact of the restrictionmodification system on transformation efficiency. We constructed the triple mutant Al01, which lacks all three annotated restriction endonucleases, and confirmed that the Al01 strain exhibits increased transformation efficiency compared to the wild-type *Caldimonas*. Our work contributes to the biotechnological domestication of *Caldimonas thermodepolymerans*, whose bioproduction potential can be now further enhanced by metabolic engineering.

## References

[1] X. Kourilova, I. Pernicova, K. Sedlar, Bioresource Technology 315 (2020) 123885.

## Acknowledgement

This project was funded by the Czech Science Foundation project No. 22-10845S.

# OW4: Cyclodextrin Polymers and Their Derivatives Containing Ionic Groups: From Synthesis and Characterization to Applications

**Heydari Abolfazl**<sup>1</sup>, Kalantarifard Shima<sup>1</sup>, El-Meligy Mahmoud A.<sup>1</sup>, Kazemi-Aghdam Fereshteh<sup>1,2</sup>, Filo Juraj<sup>2</sup>, Sadjaddi Samahe<sup>3</sup>, Omer Ahmed M.<sup>1</sup>, Mohamadnia Zahra<sup>4</sup>, Lacík Igor<sup>1</sup>

- <sup>1</sup> Polymer Institute of the Slovak Academy of Sciences, Bratislava, Slovakia; Email: abolfazl.heydari@savba.sk
- <sup>2</sup> Comenius University Bratislava, Bratislava, Slovakia
- <sup>3</sup> Iran Polymer and Petrochemical Institute, Tehran, Iran
- <sup>4</sup> Institute for Advanced Studies in Basic Science, Zanjan, Iran

## Keywords: Cyclodextrin Polymers, Ionic Groups, Synthesis

Cyclodextrin polymers (CDPs) represent a versatile class of polymers widely employed across various scientific and technological domains. Distinguished by the integration of cyclodextrins (CDs) as oligosaccharide repeating units within their polymeric network, CDPs offer a rich diversity of structures and properties. In this study, we designed straightforward methods for synthesizing charged CDP, incorporating cationic guanidine and cyanoguanidine groups, as well as zwitterionic taurine moieties, into the CDP network as shown in Figure 1. Our approach entailed the synthesis of charged CDP through the reaction of either epichlorohydrin or citric acid with charged functional groups in the presence of CD during the polymerization stages.

Preparation conditions were optimized to yield CDP exhibiting high water solubility or improved affinity for guest molecules. Comprehensive characterization employing diverse analytical techniques was undertaken to elucidate the chemical structure and determine the molar masses of the synthesized CDPs. Subsequent evaluation of the potential applicability of these polymers in drug delivery systems and 3D printing technology revealed promising prospects for their utilization in these fields.



Figure 1. Schematic representation of cyclodextrin polymers containing ionic moieties (I-CDPs) forming (a) cationic, (b) anionic, and (c) ampholytic CDPs.

## References

- [1] A. Heydari, F. Doostan, H. Khoshnood, H. Sheibani, RSC Adv 6 (2016) 33267-33278.
- [2] A. Heydari, A. Pardakhti, H. Sheibani, *Macromolecular Materials and Engineering* 302 (2017) 1600501.
- [3] L. Zongjian, Y. Lin, X. Jianing, W. Jin, F. Zeng-guo, Progress in Polymer Science 118 (2021) 101408

## Acknowledgement

This work was supported by VEGA 2/0121/23, APVV-22-0568, APVV-22-0565, and FLAG-ERA grant GRAPH-OCD, by the Slovak Academy of Sciences under the grant number FLAG ERA III/2023/808/GRAPH-OCD.

# OW5: Hybrid Materials Based on Halloysite Clay Nanotubes and Cellulose Recovered from *Egagropili*

Cavallaro Giuseppe<sup>1,2</sup>, Calvino Martina Maria<sup>1</sup>, Milioto Stefana<sup>1,2</sup>, Lazzara Giuseppe<sup>1,2</sup>

<sup>1</sup>Department of Physics and Chemistry – E. Segrè, University of Palermo, Viale delle Scienze, pad. 17, 90128 Palermo, Italy, Email: giuseppe.cavallaro@unipa.it

<sup>2</sup>Consorzio Interuniversitario Nazionale per la Scienza e Tecnologia dei Materiali, INSTM, Via G. Giusti,
9, I-50121 Firenze, Italy

## Keywords: halloysite clay nanotubes, cellulose, Egagropili, nanocomposites, geopolymers

Mixing natural clay nanoparticles with sustainable polymers represents a powerful tool to obtain composite green materials useful for packaging and building applications. In this work [1], we developed hybrid films based on halloysite nanotubes (HNTs) and cellulose recovered from Posidonia oceanica sea balls (*Egagropil*i), which are marine wastes accumulating along the Mediterranean beaches. The halloysite content of the hybrid materials was systematically varied from 30 to 80 wt%. Despite the very high amounts of clay nanotubes, the composite films exhibited macroscopic properties comparable to that of pristine cellulose.



Figure 1: Optical photos of cellulose/HNT nanocomposite films with halloysite contents of 30 and 80 wt.%. The scale bar corresponds to 1 cm.

Scanning Electron Microscopy evidenced that halloysite nanotubes form aggregates within the fibrous structure of cellulose and the microstructural characteristics of the films are affected by the cellulose/HNT composition. Accordingly, we detected that the wettability of the films can be controlled by the halloysite content. The addition of halloysite generated a thermal stabilization of cellulose and a worsening of the tensile properties. Nevertheless, the cellulose/HNT composite films showed competitive performances in terms of elasticity and mechanical resistance, although the contribution of inorganic nanotubes is predominant with respect to that of the cellulosic matrix. Cellulose/HNT films were converted into compact geopolymers by using NaOH solution for the alkaline activation of nanoclay, which was proved by thermogravimetry. The geopolymerization process induced significant increase in the rigidity and stress at break for the composite film containing the largest (80 wt.%) HNT content. Within this, Figure 2 shows the percent variations of elastic modulus and stress at breaking point of cellulose/HNT composites after the geopolymerization process.



Figure 2: Percent variations of elastic modulus (a) and stress at breaking point (b) of cellulose/HNT composites after the geopolymerization process

In conclusion, this work represents a starting step to develop composite materials through the valorization of *Egagropili*. The cellulose/HNT films can be promising for packaging applications, while the corresponding geopolymers might be employed as building materials

## References

[1] M.M. Calvino, G. Cavallaro, S. Milioto, G. Lazzara, *Environmental Science: Nano* 11 (2024) 1508.

#### Acknowledgement

This research was funded by the University of Palermo, FFR 2024 and European Union—Next Generation EU (PRIN 2022 PNRR-NANOEURO project—Cod. B53D23025300001

## **OW6: Effect of Zinc on the Properties of Portland Cement**

## Šiler Pavel<sup>1</sup>, Šilerová Iva<sup>1</sup>, Matějka Lukáš<sup>1</sup>, Novotný Radoslav<sup>1</sup>, Másilko Jiří<sup>1</sup>, Švec Jiří<sup>1</sup>

<sup>1</sup> Faculty of Chemistry, Institute of Material Chemistry, Brno University of Technology, Purkyňova 118, 61200 Brno, Czech Republic, Email: siler@fch.vut.cz

## Keywords: Portland cement, zinc, hydration, hydration accelerators

In recent years, the amount of zinc in cement and subsequently in concrete has been constantly increasing, mainly due to the use of alternative fuels and the large use of secondary raw materials containing zinc. The presence of zinc in cement significantly prolongs hydration. The aim of this work is primarily to eliminate the negative effect of zinc on cement hydration. Eliminating this effect in the future will allow the use of cement with an increased zinc content. The course of hydration was monitored using isothermal and isoperibolic calorimetry. The formation of new products and phases was monitored using differential thermal analysis and X-ray diffraction. At the same time, the morphology was studied using scanning electron microscopy with EDS microanalysis. Based on the obtained results, the possibilities of elimination of negative zinc influence using appropriately chosen hydration accelerators were found. It is precisely thanks to appropriately chosen accelerators that it is possible to obtain a material with a similar hydration time to ordinary Portland cement, but with better mechanical properties even with a higher zinc content in the mixture.

## Acknowledgement

This work was financially supported by the project GA-16646S "The elimination of the negative impact of zinc in Portland cement by accelerating concrete admixtures", with financial support from the Czech Science Foundation.

## **OW7: Wheat Bran Based Biorefinery – Proof of Concept**

## Diviš Pavel<sup>1</sup>, Pořízka Jaromír<sup>1</sup>, Slavíková Zuzana<sup>1</sup>, Nábělek Jakub<sup>1</sup>

<sup>1</sup> Brno University of technology, Faculty of Chemistry, Purkyňova 118, Brno 61200, Czech Republic, Email: divis@fch.vut.cz

## Keywords: wheat, bran, valorization, biochar, ferulic acid, protein isolate, circular economy

Wheat bran, a byproduct of the wheat milling process, is the outer layer of the wheat kernel, comprising about 14-19% of the grain. Structurally, it consists of several layers: the pericarp (outermost), testa, nucellar layers, and aleurone. The pericarp and testa are fibrous, rich in cellulose, hemicellulose, and lignin, contributing to the high dietary fiber content of bran. The aleurone layer is particularly nutrient-dense, containing proteins, lipids, vitamins (notably B vitamins), minerals (such as iron, zinc, and magnesium), and bioactive compounds like phenolic acids and flavonoids [1].

Historically considered a low-value byproduct primarily used in animal feed, wheat bran has gained recognition for its potential in human nutrition and various industrial applications. Its high dietary fiber content, particularly insoluble fiber, aids in digestive health, and its bioactive compounds have antioxidant and antiinflammatory properties, contributing to chronic disease prevention. Wheat bran can be incorporated into food products like bread, cereals, and snacks to enhance their nutritional profile [2].

Beyond its nutritional applications, wheat bran can be valorized in other innovative ways within the concept of biorefinery. The biorefinery concept involves the sustainable processing of biomass, such as wheat bran, into a spectrum of marketable products and energy [3]. Analogous to petroleum refineries, biorefineries aim to maximize the value extracted from biological materials by producing fuels, power, and high-value chemicals. This holistic approach is integral to the circular economy, which emphasizes resource efficiency and waste minimization. There are currently more than 200 biorefineries in operation in Europe, but almost two-thirds of them focus on the production of biofuels, bioethanol, or biodiesel. A complex biorefinery processing waste from the food industry into other useful products is not yet in operation, and only a few studies have validated the concept of such a biorefinery.

This work presents the concept of a biorefinery processing wheat bran, which an average-sized mill produces in the order of tens of tons per day as a byproduct of flour production. As part of this concept, the isolation of ferulic acid and proteins from wheat bran, the production of biochar from wheat bran, and the anaerobic processing of wheat bran were studied. The proposed technologies for the valorization of wheat bran were investigated in detail, verified on a small industrial scale, and the obtained products were characterized.



Figure 1: Concept of wheat bran biorefinery

## References

- [1] S. Apprich, O. Tirpanalan, J. Hell et al., LWT Food Science and Technology 56 (2014) 222.
- [2] O.O. Oluwatoyin, I.O.J. Afam, D. Beswa, Food Science and Technology 50 (2015) 2509.
- [3] F. Cherubini, G. Jungmaier, M. Wellish et al. Biofuels, Bioproducts and Biorefining 3 (2009) 534.

## Acknowledgement

The authors would like to thank the Technology Agency of the Czech Republic for supporting this research under project no. FW02020135.

## Kracalik Milan<sup>1</sup>

<sup>1</sup> Johannes Kepler University Linz, Institute of Polymer Science, Altenberger Str. 69, 4040 Linz, Austria, Email: Milan.Kracalik@jku.at

## Keywords: recycling, biodegradability, polymers

Nanotechnology is continuously expanded area of science, which contains the engineering of nanosized particles of different materials. It is the understanding and control of matter at the nanoscale, at dimensions between approximately 1 and 100 nanometers, where unique phenomena enable novel applications. Matter can exhibit unusual physical, chemical, and biological properties at the nanoscale, differing in important ways from the properties of bulk materials or individual single atoms and molecules. Some nanostructured materials are much stronger or have different magnetic, electric or insulating properties compared to other forms or sizes of the same material. They may become more chemically reactive, reflect light better, or change color as their size or structure is altered.

In the broad field of nanotechnology, polymer-matrix based nanocomposites have become an outstanding area of research and development in last decades. Nanocomposites are filled polymers with particles, where at least one dimension is in the order of nanometers. The shape of particles used in nanocomposites can be spherical, cylindrical or laminar. Maximal reinforcement is achieved using laminar or cylindrical particles because the reinforcing efficiency is highly dependent on the aspect ratio (the largest dimension divided by the smallest dimension of the particle). Conventional polymer composites are based on reinforcement of the polymer matrix by micrometer scaled particles. For example, isotactic polypropylene filled with talc, micro-ground calcium carbonate, wood powder, possibly with other suitable filler, or epoxy and polyester resins filled with mineral particles offer an advantageous combination of mechanical properties and price. However, polymeric materials reinforced by nano-scaled particles exhibit significantly higher performance (improvement in processing and application properties) already at low level of filler loading. This advantage comes from immobilization of polymer chains in close contact with inorganic filler possessing a large surface area. Using this development strategy, polymers can be improved keeping their lightweight and ductile feature. Addition of nanoscaled particles to a broad range of polymers results in significant improvement in their biodegradability and recyclability.

In this contribution, examples of biodegradable and recycled polymers reinforced by nano-scaled particles are presented and possibilities of advanced processing as well as characterization methods are introduced.

## Acknowledgement

Financial support provided by LIT Institute of Technology at Johannes Kepler University Linz, project number: LI113490001, is gratefully acknowledged.

## **OW9: Plasma Treated Water Solutions for Sustainable Agriculture**

**Kozáková Zdenka**<sup>1</sup>, Čechová Ludmila<sup>1</sup>, Trebulová Kristína<sup>1</sup>, Vozár Tomáš<sup>1</sup>, Krejsová Lenka<sup>1</sup>, Petrová Veronika<sup>1</sup>, Šindelková Kateřina<sup>1</sup>, Šťastná Kateřina<sup>1</sup>, Krčma František<sup>1</sup>

<sup>1</sup> Brno University of Technology, Faculty of Chemistry, Institute of Physical and Applied Chemistry, Purkyňova 464/118, 612 00 Brno, Czech Republic, Email: kozakova@fch.vut.cz

Keywords: non-thermal plasma, plasma-liquid interactions, reactive oxygen and nitrogen species, seed germination, plant growth, antifungal effects

Interactions of non-thermal plasma with liquids induce both physical and chemical changes leading to the formation of various reactive species containing oxygen and nitrogen with high redox potential (RONS) [1]. After the plasma application, such affected water or water solution is called plasma treated water (PTW) [2]. Due to the presence of RONS, plasma treated water gains antimicrobial properties as it induces oxidative and nitrosative stress in cells. Therefore, such stressing conditions can either inactivate microorganisms or stimulate the cell production and growth, depending on the cell kind and PTW exposition. Moreover, higher content of nitrogen species contributes to the plant growth and nutrition. Applied on seeds, PTW enhances their wettability and stimulates germination. Therefore, plasma treated water solutions offer an alternative form of a modern fertilizer with antifungal properties which can be prepared from water by minimal electric energy supply without any environmentally harmful additives and without any waste.

Composition and stability of PTW is highly dependent on the way of preparation (i.e., plasma-liquid interactions above/inside the liquid are involved), experimental conditions (preparation time, supplied power, etc.) as well as on composition of the treated liquid itself (conductivity, pH, additives, etc.) [3]. Generally, RONS produced by nonthermal plasma can be divided into the short-lived species (such as oxygen, hydrogen or hydroxyl radicals, etc.), and into the long-lived species with considerably longer lifetime in water (hydrogen peroxide, nitrites, nitrates, peroxynitrites, etc.) [1]. Especially, those long-lived species, that can be preserved in water solution for days, are utilizable in agricultural applications as nutrition agents with antimicrobial affects.

Plasma treated water solutions prepared by modified pin-hole systems generating plasma inside water volume with or without additional gas bubbling were applied on seeds and plants of *Lactuca sativa* (Figure 1), *Allium cepa*, and *Raphanus sativus*. High concentration of nitrates and

## References

- [1] P.J. Bruggemann et al., *Plasma Sources Sci. Technol.* 25 (2016) 053002.
- [2] N. Puač, M. Gherardi, M. Shiratani, *Plasma Processes and Polymers* 15 (2018) 1700174.
- [3] K. Kutasi et al., Plasma Sources Sci. Technol. 28 (2019) 095010.

#### Acknowledgement

This work was carried out within the frame of COST actions CA 19110 Plasma applications for smart and sustainable agriculture (PlAgri) and CA 20114 Therapeutical applications of Cold Plasmas (PlasTHER).

nitrites (production efficiency in the order of kJ/mg NO<sub>3</sub><sup>-</sup> or kJ/µg NO<sub>2</sub><sup>-</sup>, resp.), and sufficient concentration of hydrogen peroxide (depending on the gas addition) positively affected both seed germination as well as the growth of roots, stems and fresh biomass of all studied plants. Applied on fungi *A. niger*, PTW prevented spore creation (Figure 2). Although several microorganisms have survived, the mold reproduction was reduced.



Figure 1: Root length of Lactuca sativa exposed to plasma treated tap water or nutrient solution for 7 days.



Figure 2: Aspergillus niger after 3 weeks; left – control; right – exposed for 10 min to plasma treated physiological solution.

# OW10: Effect Evaluation of Poly-3-hydroxybutyrate Microplastics on Selected Freshwater Organisms

Zlámalová Gargošová Helena<sup>1</sup>, Procházková Petra<sup>1</sup>, Maršállková Eliška<sup>1</sup>, Kalčíková Gabriela<sup>2</sup>

- <sup>1</sup> Brno University of Technology, Faculty of Chemistry, Institute of Chemistry and Technology of Environmental Protection, Purkyňova 118, 612 00 Brno, Czech Republic, Email: zlamalova@fch.vut.cz
- <sup>2</sup> University of Ljubljana, Faculty of Chemistry and Chemical Technology, Večna pot 113, SI-1000, Ljubljana, Slovenia

## Keywords: microplastics P3HB, ecotoxicity, Lemna minor, Daphnia magna, acute and chronic effects

Microplastics with their widespread distribution are gradually becoming a global threat to the environment. Primary microplastics, which are produced in small dimensions for their intended use, are frequently used in many personal care products or rust removers and enter the environment after their application. Secondary microplastics arise from the degradation and fragmentation of larger plastic objects already present in the environment. Due to their small dimensions and persistence, microplastics are taken up by aquatic and terrestrial organisms. The resulting effects on the biota are currently the subject of intensive research. Biobased polymers have attracted considerable attention as potential substitutes for conventional polymers. These polymers are obtained from renewable resources and promise greater environmental friendliness consisting mainly of low negative effects and easy biodegradability. One of the most important groups of biobased and biodegradable polymers are polyhydroxyalkanoates. In our study, we focussed on the influence of polyhydroxybutyrate microparticles; P3HB, (ENMAT Y3000) microparticles in two size fractions – particles <63 µm and 63-125 µm. Tests on aquatic organism Daphnia magna as consumer (acute, chronic, and multigeneration tests at concentrations 0, 6.25, 12.5, 25, 50, and 100 mg)

and *Lemna minor* as producer (OECD standard test No. 221 at concentrations of 0, 10, 50, and 100 mg/L and prolonged test (12 week only at 100 mg/L) were carried out.

The L. minor exhibit no statistically significant adverse effects on the parameters studied (growth rate and photosynthetic pigment content) for either size fraction. The only statistically significant effect was root elongation with increasing P3HB concentration, perhaps as a result of stress due to nutrient depletion. During the experiment, the development of a biofilm in P3HB particles was observed, and the nutrient sorption experiment showed that the sorption capacity of P3HB was greater than that of PET. The results in D. magna demonstrated that the presence of P3HB MPs did not induce acute effects. However, in chronic and multigenerational experiments, we observed increased mortality, decreasing reproductive activity, and a slower growth rate of mother organisms, all in dependence on the concentration of P3HB MPs in suspension. Additionally, smaller MPs exhibited more pronounced effects. Both of these phenomena can be related to the ingestion of MPs, which increases with higher concentrations of MPs in suspension and smaller particle sizes. Subsequently, blockage of the digestive tract in D. magna leads to adverse consequences.

## Acknowledgement

This research was financially supported by the Ministry of Education, Youth, and Sports of the Czech Republic (project no. FCH-S-24-8591).

# OOK: Living Materials for Optoelectronics from Photosynthetic Microorganisms and Biopolymers

## Farinola Gianluca Maria<sup>1</sup>

<sup>1</sup> Università degli Studi di Bari Aldo Moro, Dipartimento di Chimica, 70125-Bari, Italy, Email: gianlucamaria.farinola@uniba.it

## Keywords: living materials, photosynthetic microorganisms, biopolymers, optoelectronics

Photosynthetic microorganisms have developed a diverse array of micro/nano structures over billions of years of evolution, finely tuned for interacting with sunlight. Utilizing these specialized structures combined with customized molecules and polymers opens up novel avenues for creating sustainable materials for optoelectronic and photonic devices [1].

The following examples will be discussed in the lecture: *i*) Photoconverters with photosynthetic bacterial enzymes. Chemical modifications are introduced to boost the performance of hybrid constructs vis-à-vis the native proteins [2] and biocompatible interfaces enable to assemble photoenzymes onto electrodes resulting in active materials for optoelectronics [3]. *ii)* Nanostructures obtained by *in vitro* and/or *in vivo* functionalization of ornate biosilica shells of diatoms unicellular algae with functional organic molecules with intriguing photonic properties [4].

*iii)* Intact photosynthetic bacteria or microalgae cells used as living materials in photoelectrochemical cells for solar energy conversion [5,6].

The lecture will discuss the logic behind designing and synthesizing the biohybrid micro/nano assemblies, highlighting the challenges raised by the controlled functionalization and integration in devices. New concepts for photoresponsive materials and devices can be envisaged by combining the biotechnological production and modification of photosynthetic microorganisms with tailored functional molecules and polymers.

## References

- [1] F. Milano, A. Punzi, R. Ragni, M. Trotta, G. M. Farinola Adv. Funct. Mater. 29 (2019) 1805521.
- [2] F. Milano, R. R. Tangorra, O. Hassan Omar, R. Ragni, A. Operamolla, A. Agostiano, G. M. Farinola, M. Trotta Angew. Chem. Int. Ed. 51(2012) 11019.
- [3] M. Di Lauro, S. la Gatta, C. A. Bortolotti, V. Beni, V. Parkula, S. Drakopoulou, M. Giordani, M. Berto, F. Milano, T. Cramer, M. Murgia, A. Agostiano, G. M. Farinola, M. Trotta, F. Biscarini, Adv. Electron. Mater. 6 (2020), 1900888.
- [4] R. Ragni, S. R. Cicco, D. Vona, G. M. Farinola Adv. Mater. 30 (2018) 1704289.
- [5] G. Buscemi, D. Vona, P. Stufano, R. Labarile, P. Cosma, A. Agostiano, M. Trotta, G. M. Farinola, M. Grattieri, ACS Appl. Mater. Interfaces 14 (2022) 26631.
- [6] L.D. de Moura Torquato, R.M. Matteucci, P. Stufano, D. Vona, G.M. Farinola, M. Trotta, M.V. Boldrin Zanoni, M. Grattieri, *ChemElectroChem* 10 (2023) 1–9.

## **OO1: Bio-Derived and Biodegradable Materials for Bioelectronics**

Turner Brendan, Twiddy, Jack, Wilkins Michael, Ramesh Srivatsan, Kilgour Katie, Domingos Eleo, Nasralla Olivia, Queener Kirstie, Reynolds James, Rivera Kristina, Martin Devon, Pozdin Vladimir, Bozkurt Alper, Lobaton Edgar, Menegatti Stefano, **Daniele Michael**<sup>1</sup>

<sup>1</sup> North Carolina State University, Campus Box 7911, Raleigh, North Carolina, USA 27695, Email: mdaniel6@ncsu.edu

## Keywords: bioelectronics, biodegradable, elastomers, nanocellulose

Mobile and distributed sensors, along with bioelectronics, are becoming increasingly prevalent due to the expanding Internet-of-Things being driven by advancements in material science, the miniaturization of electrical components, and the capabilities of edge computing.

Despite the ongoing development of soft organic and polymeric semiconductors, conventional soft circuit substrates face challenges related to processibility, sustainability, and cost. A significant area of focus lies in the advancement of sustainable materials and system designs capable of performing as effectively as traditional circuit board and newer flexible substrates, yet derived from sustainable resources.

In the pursuit of these sustainable and efficient materials for electronic applications, our research advancements have focused on a diverse array of materials, including nanocellulose, biodegradable elastomers, and nanocomposite conductors (Figure 1). These materials offer unique properties that address key challenges in electronics packaging and design, such as mechanical robustness, electrical conductivity, and environmental impact. Nanocellulose, derived from renewable biomass sources, has garnered significant attention for its high surface area, biocompatibility, and tunable properties. When integrated into electronic packaging designs, nanocellulose enhances mechanical strength and stability, while adding novel functionality such as biocompatibility, tunable gas and liquid permeation, and benign processing options.

Complementary to nanocellulose, biodegradable elastomers contribute flexibility and resilience to electronics structures, crucial for applications requiring conformal contact and durability under dynamic conditions. Biopolymer or purely synthetic biodegradable elastomers are emerging as both viable replacements for polyimide in select applications; moreover, they have been demonstrated for recyclable or compostable uses, providing for a more circular lifecycle.

This presentation will highlight our research on a range of biomaterial and nanocomposite substrates designed for bioelectronic devices. These substrates incorporate biodegradable elastomers, polysaccharides, and proteins, and they have demonstrated potential in various bioelectronic applications such as electrophysiology, recyclable nodes, and electrochemical sensing devices.



Figure 1. (a) Nanocellulose-based organic electrochemical transistors for sensing, (b) nanocellulose substrates for plant electrophysiology, (c) polysaccharide nanocomposite circuit boards, and (d) citric acid-based, biodegradable circuit boards.

## Acknowledgement

This work was sponsored by a U.S. National Science Foundation (IIS-2037328, ECCS-2231012), through an Nanosystems Engineering Research Center for Advanced Self-Powered Systems for Integrate Sensors and Technologies (EEC-1160483), and Center-to-Centre grant. This work was performed with members of the North Carolina Research Triangle Nanotechnology Network (RTNN) which is supported by the National Science Foundation (ECCS2025064) as part of the National Nanotechnology Coordinated Infrastructure (NNCI). The authors also wish to acknowledge the Molecular Education, Technology, and Research Innovation Center (METRIC).

## **OO2: Reversible Photoresponsive Systems and Materials**

## Slanina Tomáš<sup>1</sup>

<sup>1</sup> Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Flemingovo náměstí 2, Praha 160 00, Czech Republic, Email: tomas.slanina@uochb.cas.cz

## Keywords: photochemistry, organic chemistry, photoswitches, ortho-quinone methides

Light is often perceived as an immaterial elusive element that cannot transform matter. Irradiation can, however, trigger chemical species that change structure and create new chemical bonds. Therefore, light represents one of the most elegant, traceless ways to control chemical reactions and change the properties and constitution of materials.

In this contribution, we aim at molecules and molecular systems that can be activated using visible light. This activation enables a number of different processes, for example reversible selective photochemical switching of molecules between two states with different properties, formation and breaking of chemical bonds or reversible electron transfer.

Thanks to their unique properties, these molecules are widely used, for example, as light-controllable drugs, programmable molecular electronic components, affinity tags of biomolecules, photosensitive materials, functionalized polymers, organic electronics, or organic solar panels and batteries.

## References

- [1] J. Copko, T. Slanina, Chemical Communications 60 (2024) 3774.
- [2] D. Dunlop, L. Ludvíková, A. Banerjee, H. Ottosson, T. Slanina, *Journal of the American Chemical Society* 145 (2023) 21569.

## Acknowledgement

The research was funded by Funded by the European Union (ERC, SOLBATT, 101041554) and by the Czech Science Foundation (Project No. 22-20319S).

# 003: Multifunctional Nanocomposites from Naturally Derived Materials: Conductive Melanin and Crystalline Nanocellulose

Shim Bong Sup<sup>1,2</sup>

- <sup>1</sup> Department of Chemical Engineering, Inha University, 100 Inharo, Incheon, South Korea, email: bshim@inha.ac.kr; www.sbongs.com
- <sup>2</sup> Program in Biomedical Science & Engineering, Inha University, 100 Inharo, Incheon, South Korea

This presentation underscores the development of multifunctional nanocomposites that embody the principles of a circular economy, using environmentally benign materials such as synthetic melanin and crystalline nanocellulose. Our work addresses the challenges associated with the poor electrical conductivity and limited functionality of synthetic melanin by enhancing its electrochemical conductivities, optical reflectivities, and shape stability while ensuring biocompatibility. The integration of nanocellulose emphasizes its exceptional strength, biocompatibility, and contributions to

sustainability by promoting resource longevity and reducing waste. We introduce a novel synthesis method for electrically conductive synthetic melanin, opening avenues for its use in sustainable electronic devices and edible sensors that support closed-loop cycles. By advancing materials science through nature-inspired and waste-reducing innovations, this research contributes to the establishment of a circular economy, fostering the development of sustainable, multifunctional biomimetic nanocomposites.

## References

- [1] T. Eom, et al., Particle & Particle Systems Characterization 36 (2019) 1900166.
- [2] S. Kee, et al., Advanced Sustainable Systems (2021), 210056.
- [3] S., Moon, et al., Carbohydrate polymers, 254 (2021), 11470.

# OO4: Exploring End of Life Automotive Wastes as catalysts in Carbon-Carbon bond forming reactions

**Ragni Roberta**,<sup>1</sup> Cotugno Pietro,<sup>1</sup> Marangi Mariella,<sup>1</sup> Intini Gianluca,<sup>2</sup> Cangialosi Federico,<sup>2</sup> Farinola Gianluca Maria<sup>1</sup>

- <sup>1</sup> Università degli Studi di Bari Aldo Moro, Dipartimento di Chimica, 70125-Bari, Italy, Email: roberta.ragni@uniba.it
- <sup>2</sup> T&A Tecnologia & Ambiente srl S.P. 237 per Noci, 8 70017 Putignano (BA), Italy

## Keywords: automotive wastes, cross-coupling reactions, heterogeneous catalysts

End-of-life vehicles (ELVs) currently represent a valuable source of a wide variety of recyclable waste materials that deserve attention for the development of new sustainable routes to chemicals in accordance with circular economy.

In the sole European Union, more than 8 million tons of waste are yearly produced from ELVs, including 6 thousand tons of scrap automotive catalytic converters (SCATs) whose original task is to catalyze redox reactions converting toxic CO, hydrocarbons, and NOx gas products of incomplete fuel combustion in the vehicle engine into carbon dioxide, water vapor and nitrogen gases emitted from the exhaust pipe. [1,2] Scientific literature mainly reports methods of recovery of platinum group metals from SCATs via pyro- and hydro-metallurgical processes under harsh experimental conditions. [3] Despite being effective to extract precious noble metals, these processes are environmentally unfriendly, producing further toxic waste to be disposed and requiring long time and high energy consumption.

An alternative eco-friendly strategy for SCATs revalorization consists in their direct use as supported catalysts. Scientific literature shows very limited examples of investigation of the catalytic efficiency of revalued SCATs in organic reactions, these being mainly focused on reduction or oxidation processes. [4] Here we aim to demonstrate the good efficiency, general versatility and recyclability of a ELV catalytic converter regenerated by thermal treatment as heterogeneous catalyst in a series of Suzuki Miyaura cross-coupling reactions of aryl boronic acids with aryl halides.

#### References

- [1] C. M. Cova, A. Zuliani, R. Manno, V. Sebastian, R. Luque Green Chemistry 22 (2020) 1414-1423.
- [2] J. Kašpar, P. Fornasiero, N. Hickey Catalysis Today 77 (2003) 419–449.
- [3] H. B. Trinh, J. Lee, Y. Suh, J. Lee Waste Management 114 (2020) 148–165.
- [4] A. Zuliani, O. Kikhtyanin, C. M. Cova, D. Rodriguez-Padron, D. Kubička, R. Luque Adv. Sustainable Syst. 6 (2022) 2100394.

# OO5: Nanopatterning of 2D Materials by High-performance Pigment Molecules

Kocán Pavel<sup>1</sup>, Sobotík Pavel<sup>1</sup>, Cigánek Martin<sup>2</sup>, Ošťádal Ivan<sup>1</sup>, Krajčovič Jozef<sup>2</sup>

- <sup>1</sup> Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic, pavel.kocan@mff.cuni.cz
- <sup>2</sup> Brno University of Technology, Faculty of Chemistry, Materials Research Centre, Purkyňova 118, 612 00, Brno, Czech Republic

Keywords: self-assembly, scanning tunneling microscopy, metal-passivated silicon surface, highperformance pigments

Interface between an organic semiconductor and an inorganic substrate is crucial for functionality of many devices. Organic high-performance pigments, molecules such as diketopyrrolopyrroles (DPP) or epindolidiones used in this study, have a significant advantage of the facile synthesis and easy chemical modification, which resulted in their widespread use. The electronic properties can be engineered by the synthesis to match necessary requirements for the corresponding electronic devices.

As a model system we study sub-monolayer amounts of deposited organic molecules on two-dimensional (2D) metal layer grown on a silicon substrate [1]. Under clean conditions of ultra-high vacuum we study the interactions between the molecules and the substrate using scanning tunneling microscopy (STM) which allows the atomic-scale imaging (Figure 1).



Figure 1: Ordered one-dimensional chains of dithienyldiketopyrrolopyrrole molecules imaged by the scanning tunneling microscope

The 2D metal layers prepared on Si crystals often exhibit exotic properties due to strong correlation effects, such as the 2D superconductivity [2] or spin splitting of electronic states [3]. Our goal is further tuning of these **References**  exotic properties by means of self-ordered structures of organic molecules.

Organic molecules are widely used as building blocks in plethora of spontaneously growing periodic superstructures on well-defined surfaces [4]. Several types of intermolecular interactions can be involved. We have found that optimum bonding strategy when using 2D metal layers as substrates is to utilize double hydrogen bonds, as allowed by DPP or epindolidiones used in this study (Figure 2). Importantly, by modifying the side groups of the molecules we can change electronic properties of the system.

Based mostly on STM observation and density functional theory calculations, we will demonstrate our success in preparation of perfectly ordered 1D rows of the pigment molecules. We will show effect of side groups as well as of the substrate. For future, the presented approach offers a way to modify topology of electrons confined within the 2D layer.



Figure 2: Example strategies in formation of molecular structures. (a) hydrogen-bonded DPP, (b)hydrogen-bonded epindolidiones.

[1] P. Matvija, F. Rozbořil, P. Sobotík, I. Ošťádal and P. Kocán, J. Phys. Chem. Lett. 8 (2017) 4268–72.

- [2] T. Zhang et al., *Nature Physics* 6 (2010), 104.
- [3] K. Sakamoto et al., Nat. Commun. 4 (2013), 2073.
- [4] D. Goronzy et al., ACS Nano 12 (2018), 7445.

## Acknowledgement

We acknowledge support from the project MSMT CZ.02.01.01/00/22. M.C. and J.K. would like to thank the Ministry of Education Youth and Sports (MEYS) for financial support in the scope of the grant Mobility CZ-AT 8J24AT 022.

# OO6: Epitaxial Guidance of Adamantyl-Substituted Polythiophenes by Self-Assembled Monolayers

Dominik Farka<sup>1</sup>, Dominik Veselý<sup>2</sup>, Martin Ciganek<sup>2</sup>, Jozef Krajčovič<sup>2</sup>

- <sup>1</sup> Institute of Organic Chemistry and Biochemistry (IOCB), Czech Academy of Sciences; Flemingovo Náměstí 2, 160 00 Prague, Czech Republic, Email: dominik.farka@uochb.cas.cz
- <sup>2</sup> Faculty of Chemistry, Brno University of Technology (BUT), Purkyňova 118, CZ-612 00 Brno, Czech Republic

Keywords: conducting polymers, surface science, self-assembly

Charge-transport through organic materials is anisotropic in nature – control over its self-assembly therefore presents a viable pathway towards improved electronic properties. Self-assembled monolayers have been recently proven to be powerful-tools for this task as the first layer affects all of the subsequent deposition. This can completely change the materials topography and surface potential (i.e. its work-function).[1]<sup>1</sup>

Herein, we study poly(3-adamantylmethylthiophene) (PMAT, Fig.1a) [2] at the dimer and dodecamer level (Tab.1). These short oligomers display an aromatic and an adamantyl-functionality, both of which can be used to guide subsequent self-assembly.

The aromatic thiophene-subunits are expected to be the guiding moiety in the case of bare gold (Au(111), Fig.1b), while adamantyl-thiol treated gold directs towards a less disordered self-assembly pattern. Phenlythiol may, however result in a type of self-assembly in which the first layer deposited exposes an entirely adamantyl-based surface in turn, which leads to specific assembly-features.



Figure 1: (a) Chemical structure of PMAT and (b-d) possible schemes for self-assembly dependent on the employed SAM.

We compare these results with deposition on conventional substrates for optoelectronics such as unmodified glass and mica (muscovite) and compare the results accordingly.

Table 1: Properties of synthesized and employed oligos.				
MAT fractions obtained	Mn [g mol-1]	Mw [g mol-1]	Dispersity [-]	Approx. number of units [-]
2MAT	400	581	1.45	2

2 6 1 3

4 73

10

## References

[1] D.H. Apaydin, D.Farka, E.A. Schriber, M. Yeung, G. Gramse, N.S.Sariciftci, D. Eder, J.N.Hohman, ACS Appl.Nano. Mater. 5 (2022).

10MAT

552

[2] J. Jančík, J. Pospíšil, M. Kratochvíl, J.Truksa, D. Altamura, C.Giannini, M. Weiter, D. Blasi, V. Lukeš, E.D. Glowacki, J. Krajčovič, Polymer 258 (2022), 125274.

#### Acknowledgement

DF acknowledges J.A.A.W. Elemans (Radboud University Nijmegen) and Eva Kaletová (IOCB) for scientific discussions and the financial support of the IOCB through the IOCB fellowship ("Covalent epitaxy") and Dr. Ivo Starý for accomodation within his research group. DV, MC, and JK acknowledge the financial support of the Ministry of Education Youth and Sports (MEYS; projects 95p3 and 8J24AT 022)

## 007: Colour-Tuneable Solid-State Fluorescence of Push–Pull Substituted 2,5-Diphenyl-Stilbenes

Vala Martin<sup>1</sup>, Rastislav Smolka<sup>1</sup>, Stanislav Luňák<sup>1</sup>, Karel Pauk<sup>2</sup>, Martin Weiter<sup>1</sup>, Aleš Imramovský<sup>2</sup>

- <sup>1</sup> Brno University of Technology, Faculty of Chemistry, Purkyňova 464/118, 612 00 Brno, Czech Republic, Email: vala@fch.vut.cz
- <sup>2</sup> University of Pardubice, Faculty of Chemical Technology, Studentská 95, 532 10 Pardubice, Czech Republic

## Keywords: Organic fluorophores, deep-red emission, fluorescent nanoparticles, excimer design

This study focuses on the solid-state fluorescence (SSF) of eight DPA-DPS-EWG derivatives. DPA (diphenylamino) and DPS (2,5-diphenyl-stilbene building block) are the basic components of these derivatives, while EWG (electron-withdrawing group) allows tuning the electronic properties of the molecules, see the Figure 1. Variations in EWG strength allowed tuning of the LUMO energy over a range wider than 1 eV, while HOMO energy changes were less than 0.1 eV.

The fluorescence maxima in dichloromethane ranged between 483 and 752 nm, indicating the wide range of colour tunability of these derivatives. For all derivatives, the monoexponential decay with photoluminescence quantum yield (PLQY) higher than 35 % was observed. This indicates that these molecules can emit light efficiently.

The six derivatives with SSF PLQY higher than 10% in polycrystalline powder form covered the range from 475 to 733 nm. This shows that these molecules are capable of efficiently emitting light also in the solid state. Three components of the multiexponential decay of SSF, obtained by time-resolved fluorescence spectroscopy, were attributed to the migration of excitons into nonfluorescent traps, monomer-like fluorescence, and aggregate fluorescence. This suggests that different mechanisms contribute to the overall fluorescence behaviour of these molecules in the solid state.

The nature of the emitting aggregates was assessed by quantum chemical modelling based on TD-DFT calculations performed on dimeric arrangements obtained by X-ray diffractometry of single crystals. Exciton localisation either on a monomer (in J-like packing) or a stacked dimer (for Haggregates) was found to be effective for improving the overall SSF PLQY through an avoidance of exciton migration to the quenching sites by a self-trapping process. The highest SSF PLQY (35%) was found for the red emission of DPA-DPS-CMV (CMV = cyanomethylvynylene) with the deepest trap, localised on an electronically isolated stacked dimer, causing delayed fuorescence with a lifetime more than 5 times longer compared to the monomer fuorescence in solution.

It was found that DPA-DPS-DCV (DCV = dicyanovinylene) showed the formation of a polymorph with very intense solid-state fluorescence (PLQY 32 %) in the deep red region (maximum 733 nm). The anomalous nature of the photoluminescence spectral position to the other molecules in set and partial CT character in stacked dimer arrangement pointed to the excimer character of this far-red emission.

These results suggest that limiting exciton migration is one of the few general ways to obtain highly luminescent poly- and nanocrystalline organic solids. Possibility to influence this effect is important for the development of new materials for optoelectronic devices such as organic light emitting diodes (OLEDs) and organic solar cells. This research provides insights into the relationship between the solid-state structure and luminescent properties of these materials and opens new possibilities for their practical applications.



Figure 1: Notations of the compounds under study.

## Acknowledgement

The work was supported by the Czech Science Foundation, project no. 24-10479S.

# **OO8: Graphitic Carbon Nitride Coatings: Synthesis, Processing and Environmental Applications**

**Dzik Petr<sup>1</sup>**, Patakyová Sylvia<sup>1</sup>, Veselý Michal<sup>1</sup>, Stavárek Petr<sup>2</sup>, Klusoň Petr<sup>2</sup>, Homola Tomáš<sup>3</sup>, Zažímal František <sup>3</sup>

- <sup>1</sup> Faculty of Chemistry, Brno University of Technology, Purkyňova 118, 612 00 Brno, Czech Republic, Email: dzik@fch.vut.cz
- <sup>2</sup> Institute of Chemical Process Fundamentals of the Czech Academy of Sciences, Rozvojová 2/135, 165 02 Prague, Czech Republic
- <sup>3</sup> Department of Plasma Physics and Technology, Faculty of Science, Masaryk University, Kotlářská 267/2, 611 37 Brno, Czech Republic

## Keywords: graphitic carbon nitride, wet coating, solution processing, templating, pore forming

Since its discovery in 2006, graphitic carbon nitride (GCN) has attracted significant interest due to its photocatalytic activity, despite the fact that the substance is not new [1, 2]. GCN is composed of tri-s-triazine rings cross-linked by trigonal N atoms [3]. One of its main advantages is that it is a metal-free medium-band-gap semiconductor with high thermal and chemical stability and a tunable electronic structure. Its properties make it a promising material for various applications. The electronic band gap of GCN is approximately 2.7 eV, which is lower than that of the photocatalytic standard, titanium dioxide (TiO2), which is 3.2 eV [3]. Based on its electron structure, GCN should be capable of oxygen and hydrogen evolution through water splitting. Additionally, GCN is easy and inexpensive to synthesize, making it an attractive semiconductor for larger scale use.

This report outlines the fabrication and properties of durable GCN coatings with enhanced porosity. The adhesion and cohesion of these coatings are ensured by a proprietary oligomeric siloxane binder [4]. GCN was synthesized from a melamine-cyanurate complex. The crude GCN was wet ball-milled in isobutanol to prepare a suspension of GCN particles with a narrow size distribution suitable for coating. Following the milling process, a coating formulation was prepared by adding a variable amount of oligomeric siloxane binder and a sacrificial pore-forming agent, camphor. The plain soda-lime glass slides and FTO substrates were coated using the doctor blade technique. The coated substrates were heated to 80 °C under reduced pressure, resulting in the quantitative sublimation of camphor from the layer. This process left voids, the shape of which was strongly dependent on the concentration of camphor.

Mechanical, physical and chemical properties of fabricated coatings were investigated in detail by various methods and photocatalytic activity was evaluated with several model pollutants in order to determine the optimal pore-forming agent content. We have shown that the porous texture improves the photocatalytic activity by enhancing the mass transfer as well as light penetration into the catalyst layer

## References

- [1] F. Goettmann et al., Angewandte Chemie-International Edition 45 (2006) 4467-4471.
- [2] F. Goettmann et al., *Chemical Communications* 43 (2006) 4530-4532.
- [3] X. C. Wang, S. Blechert, M. Antonietti, Acs Catalysis 2 (2012). 1596-1606.
- [4] T. Svoboda, M. Veselý, R. Bartoš, T. Homola, P. Dzik, Catalysts 11 (2021) 50

## Acknowledgement

This work has received financial support from the Czech Science Foundation through project 23-06843S.

## Irimia-Vladu Mihai<sup>1</sup>

<sup>1</sup> Johannes Kepler University Linz, Institute of Physical Chemistry, Linz Institute for Organic Solar Cells, TNF Tower, 8th floor, Altenberger Str. Nr. 69, 4040 Linz, Austria Email: mihai.irimia-vladu@jku.at

## Keywords: natural dielectrics, nature-origin materials, field-effect transistors

Organic electronics has an immense potential for the development of products that are both sustainable and environmentally friendly. In this oral presentation, a large list of natural origin dielectric materials is introduced and explored in the fabrication of field effect transistors *i.e.* lignins [1], and celluloses [2], resins [3,4] gums, waxes, alkaloids, nucleobases [5], etc.

The thin natural organic dielectric materials listed above were used either as stand-alone insulator layers or as capping layers for the electrochemically grown aluminum oxide on the top of the gate electrode. We assess and establish the specific dielectric properties of each material, *i.e.* impedance characteristics, dielectric constant, and breakdown field. Finally, we demonstrate their efficient application as gate dielectric materials for organic field-effect transistors (OFETs), with both p-type and n-type organic semiconductor molecules, *i.e.* pentacene and fullerene, C<sub>60</sub>. The dielectric materials investigated in this study are practical alternatives for the fabrication of sustainable, "green" electronics, considering their natural origin and wide availability, their low cost of production, their low toxicity, inherent biodegradability, and finally the most important aspect, their ultimate performance, and stabilityreliability in practical devices.

Apart for the outstanding dielectric and film forming properties presented in this lecture, it is worth noting that all the above-mentioned natural dielectrics are inherently, biocompatible (even edible) and have well known medical properties. Thus, this class of dielectrics may find in future applications in the branches of science where dielectric materials are part of bio-integrated electronics.

## References

- [1] R. D'Orsi, V. V. Irimia, J. J. Lucejko, B. Kahraman, Y. Kanbur, C. Yumusak, F. Babudri, M. Irimia Vladu, A. Operamolla, *Adv. Sust. Syst.* 6 (2022) 2200285.
- [2] A. Petritz; A. Wolfberger; A. Fian; M. Irimia-Vladu; A. Haase; H. Gold; T. Rothländer; T. Griesser; B. Stadlober, *Appl. Phys. Lett.* 103 (2013) 153303.
- [3] J. Ivić, A. Petritz, C. V. Irimia, B. Kahraman, Y. Kanbur, M. Bednorz, C. Yumusak, M. A. Aslam, A. Matković, K. Saller, C. Schwarzinger, W. Schühly, A. I. Smeds, Y. Salinas, M. Schiek, F. Mayr, C. Xu, C. Teichert, M. Osiac, N. S. Sariciftci, B. Stadlober, M. Irimia-Vladu, *Adv. Sust. Syst.* 6 (2022) 2200234.
- [4] M. E. Coppola, A. Petritz, C. V. Irimia, C. Yumusak, F. Mayr, M. Bednorz, A. Matkovic, M. A. Aslam, K. Saller, C. Schwarzinger, M. D. Ionita, M. Schiek, A. I. Smeds, Y. Salinas, O. Brüggemann, R. D'Orsi, M. Mattonai, E. Ribechini, A. Operamolla, C. Teichert, C. Xu, B. Stadlober, N. S. Sariciftci, M. Irimia-Vladu, *Global Challenges* 7,(2023) 2300062.
- [5] M. Irimia-Vladu, P. A. Troshin, M. Reisinger, L. Shmygleva, Y. Kanbur, G. Schwabegger, M. Bodea, R. Schwödiauer, A. Mumyatov, J. W. Fergus, V. F. Razumov, H. Sitter, N. Serdar Sariciftci, S. Bauer, Adv. Funct. Mater. 20 (2010) 4069–4076.

## Acknowledgement

Financial support from the project "EINSTEIN", grant number. 101136377 (HORIZON-WIDERA-2023-ACCESS-03) is gratefully acknowledged. We also gratefully acknowledge the Wittgenstein Prize of the Austrian Foundation of Advancement of Science (FWF) for Prof. Serdar Sariciftci (project number Z 222-N19).

## **OO10: Novel PEDOT-Based Hydrogel for Bioelectronic Applications**

**Tumová Šárka**<sup>1</sup>, Malečková Romana<sup>1</sup>, Marková Aneta<sup>1</sup>, Pospíšil Jan<sup>1</sup>, Smilek Jiří<sup>1</sup>, Pešková Michaela<sup>2, 3</sup>, Kubáč Lubomír<sup>4</sup>, Víteček Jan<sup>2</sup>, Vala Martin<sup>1</sup>, Weiter Martin<sup>1</sup>

- <sup>1</sup> Faculty of Chemistry, Brno University of Technology, Purkyňova 464/118, 612 00 Brno, Czech Republic, Email: Sarka.Tumova@vut.cz
- <sup>2</sup> Department of Biophysics of Immune System, Institute of Biophysics of the Czech Academy of Sciences, Královopolská 135, 612 65 Brno, Czech Republic
- <sup>3</sup> Department of Biochemistry, Faculty of Science, Masaryk University, Kamenice 5, 625 00 Brno, Czech Republic
- <sup>4</sup> Centre for Organic Chemistry, Rybitví 296, 533 54 Rybitví, Czech Republic

Keywords: PEDOT, conductive hydrogel, impedance spectroscopy, cells, OECT, biocompatibility

Organic bioelectronics emerged as a potential revolution in medical care as it enables highly efficient individualized therapy with reduced side effects compared to conventional pharmacological treatment.

Bioelectronic devices consist of several components, the crucial one, that determines the performance of the whole device, is active material. Active material acts as a converter of cell communication into the form of an electrical signal and *vice versa*. Therefore, there are high demands on active materials to obtain devices capable of precise diagnostic and highly effective therapy. The main parameters the active material should meet are (i) high biocompatibility, to avoid adverse reactions of the living organism, (ii) a suitable combination of ionic and electronic conductivity, to effectively transform the cell communication that occurs in the form of ionic signals into the electrical signal and (iii) suitable mechanical properties not to cause damage to the soft biological tissues.

Most bioelectronic devices use the active material in the form of thin film, which is not suitable for contact with living cells due to the significant differences in mechanical properties. Thin films are dry and rigid structures and their connection to the wet, soft and very dynamic biological tissues often leads to the damage of both, the bioelectronic device as well as living tissue.

Hydrogels are considered an ideal environment for living tissues as their properties are very similar to those of extracellular matrix. However, conventional hydrogels are not suitable for bioelectronic applications as they lack ionic and electronic conductivity. Several research groups put great efforts to overcome this drawback and prepared mixed conductive hydrogels combining a conductive component (e.g. metal nanoparticles or conductive polymers) and the conventional non-conductive hydrogel matrix. However, this approach always suffers from the trade-off between suitable mechanical properties given by hydrogel and appropriate conductivity given by dopant.

Recently, it was shown that it is possible to prepare a pure conductive PEDOT hydrogel, which was a breakthrough discovery, as such structure possesses both, suitable mechanical and electrical properties [1]. Since then, a lot of attention has been dedicated to this topic as it can represent a significant shift to more effective bioelectronics devices and expand their application possibilities.

Here, we present the preparation of novel pure conductive hydrogel based on polymer composite PEDOT:DBSA. Prepared hydrogel exhibits improved biocompatibility compared with PEDOT:PSS, which constitutes the golden standard in this field, tunable mechanical properties and suitable electrical properties for bioelectronic applications. The suitability of PEDOT:DBSA hydrogel to form an active material in bioelectronic devices was proved by its utilization in an organic electrochemical transistor (OECT), which showed typical transistor behavior. Such hydrogel-based OECT is, to the best of our knowledge, unique and can provide a knowledge base for the next generation of highly effective hydrogel bioelectronics.

#### References

[1] S. Zhang, Y. Chen, H. Liu et al, Advanced Materials 32 (2020).

#### Acknowledgement

The authors acknowledge that the work was supported by the Czech Science Foundation, project No. 21-01057S.

# OS1: Chemically Responsive Melanin-Like Polymers for Living Cell Display Technology

**Digregorio Alessandro**<sup>1</sup>, Flemma Annarita<sup>1</sup>, Vicente-Garcia Cesar<sup>1</sup>, Cotugno Pietro<sup>1</sup>, Cicco Stefania Roberta<sup>2</sup>, Ragni Roberta<sup>1</sup>, Vona Danilo<sup>3</sup>, Farinola Gianluca Maria<sup>1</sup>

- <sup>1</sup> University of Bari, Department of Chemistry, Via Orabona 4, Bari, 70125, Italy Email: alessandro.digregorio@uniba.it
- <sup>2</sup> CNR-ICCOM, Institute of Organometallic Chemistry, Via Orabona 4, Bari, 70125, Italy
- <sup>3</sup> University of Bari, Department of Soil, Plant and Food Sciences, Via Orabona 4, Bari, 70125, Italy

## Keywords: organic biopolymers, polydopamine, microalgae, diatoms, living materials, bioremediation

Living cells can work as natural platforms for chemical functionalization, exhibiting a multitude of functional groups and biomolecules. The addition of chemical functionalities onto living cells creates an engineered surface enabling bacteria, yeasts, microalgae and even mammalian cells, to recognize their environment. Thus, they can incorporate both *cell-to-cell* and *cell-to-environment* interactions useful for various purposes, from biomedicine to industrial applications [1].

On this topic, scientific research has been focused on developing methods to decorate living microalgae using sticky, melanin-like organic polymers. Recently, polydopamine (PDA), a biocompatible polymer based on poly-hydroxy-indole species, has been used to create selfassembling coatings on living cells. For instance, this has allowed microalgae to continue living and dividing while increasing their resistance to harsh environmental conditions [2].

This technology is simple, one pot, and reliable, yielding a highly reactive surface capable to interact with other exogenous functional groups to change the chemical reactivity on the living cell surfaces.

During self-polymerization, dopamine monomer (DA) is first oxidized to form reaction intermediates such as the indole species (5,6-dihydroxyindole, DHI and 5,6-indolequinone) which can react with amino group through Michael addition or Schiff-base reaction.

Our studies are focused on the co-polymerization of DA with aminophenylboronic acids in ammonia solution. The obtained boronic-bearing luminescent polymer can coat living cells with high density glycocalyx, *via* an esterification reaction of the boronic unit with the vicinal diol functionalities of the saccharides. Moreover, the presence of free boronic moieties on functionalized cells let them act as living platforms displaying further chemical linking properties.

Another strategy is the co-polymerization of DA with polyethyleneimines, for the creation of living cells externally decorated with active amino groups useful for the removal of pollutants from aqueous environment (e.g. emerging small molecules, microplastics) [3].

Finally, redox responsive melanin-like polymers were also synthesized via co-polymerization of DA with cysteamine, to add disulfide bridges to the polymer bulk. Thus, these bioinspired polymers can be cleaved with specific reduction reactions, making them re-usable and recyclable systems in the field of bioremediation.

In this work, we demonstrate the reliability of coating polymerization on living cells, which has a very limited impact on their viability, while conferring them several new and different functionalities, potentially useful for many technological applications.

## References

[1] M. Lo Presti, D. Vona, R. Ragni, S.R. Cicco, G.M. Farinola, MRS Communications 11 (2021) 213-225.

- [2] D. Vona, S.R. Cicco, R. Ragni, C. Vincente-Garcia, G. Leone, M.M. Giangregorio, F. Palumbo, E. Altamura, G.M. Farinola, *Photochemical & Photobiological Sciences* 21 (2022) 949-958.
  - [3] A. Aresta, S.R. Cicco. D. Vona, G.M. Farinola, C. Zambonin, Separations 9(8) (2022) 194.

# OS2: Tissue Engineering Scaffolds Prepared by Supercritical Carbon Dioxide Foaming from Polyhydroxyalkanoates

Šindelář Jan<sup>1,2</sup>, Přikryl Radek<sup>1</sup>, Massera Jonathan<sup>2</sup>

- <sup>1</sup> Brno University of Technology, Faculty of Chemistry, Purkyňova 464/118, 612 00, Brno Email: jan.sindelar@vut.cz
- <sup>2</sup> Tampere University, Tampere, Finland

Keywords: polyhydroxyalkanoates, tissue engineering, pressure-induced phase separation, supercritical CO<sub>2</sub>, bioactive glass

Biodegradable polyesters such as polylactide (PLA), polyglycolide (PGA), polycaprolactone (PCL) and their copolymers or blends are among the most commonly used materials for tissue engineering scaffolds. They can be processed by traditional melt processing methods such as extrusion or injection moulding. After implantation, they degrade by hydrolysis and are eventually completely resorbed, and the degradation products are metabolised [1,2].

Polyhydroxyalkanoates are polymers synthetized by various bacteria, which use them as energy and carbon storage. Even though they are of natural origin, they are thermoplastics with properties similar to biodegradable polyesters, and they also degrade by hydrolysis after The used implantation. most commonly polyhydroxyalkanoate is poly-3-hydroxybutyrate (P3HB). The main advantage of P3HB is the fact that its monomer, the  $\beta$ -hydroxybutyric acid is one of the keto bodies. It is naturally present in most human tissues. It can be used as an energy source, unlike lactic acid, the degradation product of PLA, which needs to be metabolised and removed from the body. β-hydroxybutyric acid is also less acidic and therefore doesn't acidify the surrounding environment of the scaffold so much as lactic acid, which may lead to better healing and creation of new tissue [1,3,4].

P3HB is however highly crystalline, brittle, and can be hard to process due to a narrow window between melting

and degradation temperature. However, its copolymers with other polyhydroxyalkanoates, such as poly-4hydroxybutyrate, poly-3-hydroxyvalerate, and poly-3hydroxyhexanoate offer a wide range of properties that can be tailored by using different ratios of monomers and by blending them with other polyhydroxyalkanoates. They are less crystalline or completely amorphous. Their melting or softening temperature is lower, while the degradation temperature remains similar. The mechanical properties can range from elastomers to stiff and brittle materials [1,2,5].

In this work, porous scaffolds were prepared by pressure-induced phase separation using supercritical CO<sub>2</sub> as a foaming agent. Scaffolds were prepared from poly-3co-4hydroxybutyrate (P3,4HB), a blend of poly-3hydroxybutyrate-co-3-hydroxyhexanoate with poly-3hydroxybutyrate (PHBH) and from a composite of PHBH and phosphate bioactive glass. They were compared to scaffolds prepared from PLA and PCL. A wide range of properties was achieved. Especially notable is the highly elastic P3,4HB foam with 20x lower elastic modulus than PCL, which is the most elastic of commonly used biodegradable polyesters. This shows the potential of polyhydroxyalkanoates in various tissue engineering applications. P3,4HB has great potential in the regeneration of soft tissues, while the PHBH and bioactive glass composite can be used for bone regeneration.

## References

[1] C.S.K. Reddy, R. Ghai, Rashmi, V.C. Kalia, *Bioresource Technology* 87 (2003) 137–146.

[2] J. Lim, M. You, J. Li, Z. Li, *Materials Science and Engineering: C* 79 (2017) 917–929.

[3] M.L. Bruss, *Lipids and Ketones*, in: J.J. Kaneko, J.W. Harvey, M.L. Bruss (Eds.), Academic Press, San Diego, USA, 2008, 81–115.

[4] C. Wang, T. Chang, H. Yang, M. Cui, Food Control 46 (2014) 525–531.

[5] K. Eraslan, C. Aversa, M. Nofar, M. Barletta, A. Gisario, R. Salehiyan, Y.A. Goksu, *European Polymer Journal* 167 (2022) 111044.

# OS3: Biodegradable Nanocomposites Based on the Ecovio<sup>®</sup> (PBAT and PLA): Thermal and Rheological Properties

## Kostenko Mariia<sup>1,2</sup>, Stetsyshyn Yurij<sup>2</sup>, Kracalik Milan<sup>1</sup>

- <sup>1</sup> Johannes Kepler University Linz, Institute of Polymer Science, Altenberger Str. 69, 4040 Linz, Austria, Email: mariia.kostenko@jku.at
- <sup>2</sup> Lviv Polytechnic National University, 3/4 St. Yura square, 79013 Lviv, Ukraine

Keywords: polylactide, Ecovio<sup>®</sup>, nanocomposites, biodegradable polymers, mechanical properties, thermal properties

Improving the properties of polymeric materials is an urgent task that allows increasing their operational properties, improving technological parameters or accelerating the time of biodegradation [1,2]. This trend has become especially relevant in recent decades when traditional synthetic polymers have been replaced by their biodegradable and often bio-based counterparts. Biodegradable polymers, which are already produced on an industrial scale, are of particular interest. Among them is compostable polymer blend Ecovio® which consists of the BASF polymer Ecoflex®, polylactid acid (PLA) and other additives [2]. In contrast to simple starch-based bioplastics, Ecovio® is more resistant to mechanical stress and moisture. Ecoflex® is polybutylene adipate-coterephthalate - a completely biodegradable statistical copolyester based on the fossil monomers 1,4butanediol, adipic acid and terephthalic acid. In turn, PLA is one of the most promising biodegradable polymers, gaining increasing popularity due to its environmental properties and potential use in various industries such as packaging or biomedical products.

One of the current trends in the development of advanced nanocomposites is the inclusion of nano-

additives in their structure, which potentially provide them with improved mechanical, thermal and barrier properties compared to pure polymers. In this study, Ecovio®-based nanocomposites were fabricated using functionalized montmorillonite clay nanofillers, including modified (3-aminopropyl)triethoxysilane, and grafted polymer brushes (poly(butyl methacrylate) (PBMA) or poly(butyl acrylate) (PBA)) [3].

The obtained Ecovio® nanocomposites were intensively characterized. These studies include the analysis of heat resistance and thermal properties of composites using DSC and TGA. A particularly important aspect of research is the use of rheological methods to determine the characteristics of nanocomposites. This approach makes it possible to evaluate the viscoelastic properties of polymer composites subjected to mechanical stress. Rheological studies contributed to the determination of the structural and dynamic properties of the polymer matrix, as well as the influence of nanoparticles on its behavior [4].

The research results substantiate the potential of manufacturing nanocomposites based on Ecovio<sup>®</sup> as highly efficient materials.

## References

- [1] N. Chatiras, P. Georgiopoulos, A. Christopoulos, E. Kontou, Polymer Composites 40(11) (2019) 4340.
- [2] K. Hamad, M. Kaseem, M. Ayyoob, J. Joo, F. Deric, Progress in Polymer Science 85 (2018) 83.
- [3] M. Kostenko, Y. Stetsyshyn, K. Harhay, Y. Melnyk, V. Donchak, Z. Gubriy, M. Kracalik, J. of Applied Polymer Science 141(25) (2024) e55543.

[4] M. Kracalik, S. Laske, A. Witschnigg, C. Holzer, Rheol. Acta 50 (2011) 937.

## Acknowledgement

We would like to express our gratitude for the financial support provided by the LIT Institute of Technology at Johannes Kepler University Linz, project number: LIT-2022-11-SEE-123. Furthermore, we would like to acknowledge the financial support from OeAD-GmbH, Ernst Mach Grant, EM UKR/Batch II, Nr. MPC-2022-04295 and Mobility Program Nr. MPC-2021-01858.

# OS4: Green Energy Production Using Flavin-inspired Photosensitisers

**Ivanová Lucia**<sup>1</sup>, Truksa Jan<sup>1</sup>, Whang Dong Ryeol<sup>2</sup>, Yumusak Cigdem<sup>3</sup>, Sariciftci Niyazi Serdar<sup>3</sup>, Krajčovič Jozef<sup>1</sup>

- <sup>1</sup> Brno University of Technology, Faculty of Chemistry, Purkyňova 118, 612 00 Brno, Czech Republic, Email: xcivanova@vutbr.cz
- <sup>2</sup> Department of Advanced Materials, Hannam University, 1646 Yuseong-Daero, Yuseong-Gu, Daejeon 34054, Republic of Korea
- <sup>3</sup> Linz Institute for Organic Solar Cells (LIOS), Institute of Physical Chemistry, Johannes Kepler University Linz, Altenberger Straße 69, 4040 Linz, Austria

Keywords: artificial photosynthesis, flavin, photosensitiser, hydrogen evolution reaction

Green hydrogen is considered a clean, sustainable energy vector with the potential to play a crucial role in decarbonising energy systems. Nowadays, it is mainly produced through water electrolysis using renewable energy sources such as wind and solar power.

Artificial photosynthesis has recently shown a new strategy for producing green hydrogen and strategic and economically valuable substances like methanol or methane. It mimics natural photosynthesis and thus stores the power of such renewable energy sources in the chemical bonds.

One of the challenging problems is the development of new photosensitisers, the light-harvesting antennae. This research focuses on the design and synthesis of novel vitamin B2-inspired metal-free organic photosensitisers that are suitable for molecular photocatalytic systems.

In our previous studies, flavins have been found to possess unique properties that make them an attractive candidate for photocatalytic hydrogen evolution [1,2].

For the presented study, we have chosen a flavin photosensitiser (Figure 1) that absorbs light in the visible part of the spectrum. The choice was made based on suitable levels of frontier molecular orbitals, and the possibility of long-lived triplet state formation was predicted [3]. This system consists of a flavin photosensitiser for light capture and electron transfer and a platinum co-catalyst providing active sites for the reaction. A sacrificial reagent was used to facilitate the oxidative half-reaction. The optimal ratio of photosensitiser to co-catalyst was determined. The system demonstrated continuous hydrogen production over 29 hours, indicating sufficient photostability (compared to Eosin Y) and reproducibility through repeated measurements [3]. This work highlights the potential of flavins as a sustainable and tunable platform for green hydrogen production, offering a promising alternative to traditional materials.



Figure 1: Molecular structure of flavin photosensitiser

## References

- [1] J. Richtar, P. Heinrichova, D. Apaydin, V. Schmiedova, C. Yumusak, A. Kovalenko, M. Weiter, N.S. Sariciftci, J. Krajcovic, *Molecules* 23 (2018) 2271.
- [2] J. Richtar, L. Ivanova, D.R. Whang, C. Yumusak, D. Wielend, M.Weiter, M.C. Scharber, A. Kovalenko, N.S. Sariciftci, J. Krajcovic, *Molecules* 26 (2021) 27.
- [3] L. Ivanová, J. Truksa, D.R. Whang, N.S. Sariciftci, C. Yumusak, J. Krajcovic, ACS Omega 9 (2024), 5534–5540.

## Acknowledgement

The authors thank the project FCH-S-24-8592, the Austrian Agency for International Cooperation in Education and Research (OEAD-GmbH, WTZ, CZ01/2020, 8J20AT025) and FWF Mobility CZ-AT project 8J24AT022. LI thanks the Brno City Municipality (Brno Ph.D. Talent Scholarship) for her financial support.

# OS5: Acrylated and Itaconated Plant Oils as Eco-Friendly Monomers for Emulsion Polymerisation

Kolář Martin<sup>1</sup>, Machotová Jana<sup>1</sup>, Podzimek Štěpán<sup>1,2</sup>, Honzíček Jan<sup>1</sup>, Kocián David<sup>3</sup>

- <sup>1</sup> Institute of Chemistry and Technology of Macromolecular Materials, Faculty of Chemical Technology, University of Pardubice, Studentská 573, 532 10 Pardubice, Czech Republic, email: st51413@upce.cz
- <sup>2</sup> Synpo, a. s., S. K. Neumanna 1316, 532 07 Pardubice, Czech Republic
- <sup>3</sup> Department of Physical Chemistry, Faculty of Chemical Technology, University of Pardubice, Studentská 573, 532 10 Pardubice, Czech Republic

## Keywords: emulsion polymerisation, coating, acrylic latex, camelina oil

Emulsion polymerisation is a widely used technique for multiple applications, such as bulk polymers and latex coating systems. A variety of monomers can be utilised in emulsion polymerisation; however, the vast majority are petroleum-based. The growing concern evokes new research and a search for more eco-friendly alternatives. Promising materials are plant oils with a high content of unsaturated fatty acids. However, the double bonds present in their molecules are not reactive enough to successfully perform in an emulsion polymerisation and they have to be modified by introducing more reactive moieties [1].

Acrylated derivatives, prepared by epoxidation and subsequent acrylation, have emerged as valuable and relatively eco-friendly materials [2]. Unfortunately, their manufacturing process requires a non-negligible amount of petroleum-based acrylic acid. Additionally, acrylic acid has allergenic and irritation potential.

The replacement of acrylic acid with itaconic acid is a possible solution to these inconveniences. Itaconic acid is produced by fermentation of carbohydrates. Its solid-state also solves the problems that arise from the volatility of acrylic acid. Since itaconic acid contains two carboxylic groups, it has to be modified to mimic the acrylic acid structure. In this work, we used camelina oil, derived from the cruciferous plant *Camelina sativa*, to obtain acrylic monomers using transesterification, epoxidation, and acrylation or itaconation. For the purpose of itaconation, we synthesised monomethyl itaconate, which we further used as an alternative for acrylic acid in the same synthesis. The reaction scheme (Figure 1) is portrayed on a methyl ester of oleic acid. These monomers were then copolymerised in a conventional semi-continuous

emulsion polymerisation with commercial acrylic monomers.



Figure 1: Itaconation of camelina oil

Molar mass measurements of the latex copolymers showed the formation of an ultrahigh molecular weight fraction due to the presence of multi-acrylated/itaconated ingredients from the bio-based monomers. An increase in water repellency and resistance against water-whitening in the coating samples was observed. Long fatty acid chains were responsible for this phenomenon, although the presence of hydroxyl groups (from oxirane rings) significantly reduced this effect.

In conclusion, acrylation and itaconation are effective methods that can be used to modify various plant oils, as well as manufacturing by-products (such as tall oil) into valuable eco-friendly materials for the polymeric industry.

#### References

[1] J.S. Neves, L.F.Valadares, F. Machado, Colloids and Interfaces 2 (2018) 46.

[2] M. Kolář, J. Honzíček, Š. Podzimek, P. Knotek, M. Hájek, L. Zárybnická, J. Machotová, *Journal of Materials Science* 58 (2023) 15558–15575.

### Acknowledgement

This work was supported through project No. UPA/SG321005.

## OS6: Macro- and Microrheological Characterization of Cerebrospinal Fluid

**Bauer Thessa-Carina**<sup>1</sup>, Bradt Elke<sup>1</sup>, Hild Sabine<sup>1</sup>, Gruber Andreas<sup>2</sup>, Rossmann Tobias<sup>2</sup>, Ruiz-Navarro Francisco<sup>2</sup>, Oberndorfer Johannes<sup>2</sup>, Stefanits Harald<sup>2</sup>, Kracalik Milan<sup>1</sup>

- <sup>1</sup> Johannes Kepler University Linz, Institute of Polymer Science, Altenberger Str. 69, 4040 Linz, Austria, Email: thessa-carina.bauer@jku.at
- <sup>2</sup> Kepler University Hospital, Department of Neurosurgery and Johannes Kepler University Linz, Faculty of Medicine, Clinical Research Institute for Neurosciences, Wagner-Jauregg-Weg 15, 4020 Linz, Austria

Keywords: rheology, viscosity, characterization, cerebrospinal fluid, hydrocephalus

Rheology is considered to characterize the flow behavior of different fluent macromolecular materials. In medical science rheology has little awareness. Biological fluids are aqueous solutions containing several macromolecules, as proteins among others, which are responsible for a specific flow behavior. Some studies have been conducted on synovia and blood. This study focuses on cerebrospinal fluid (CSF) especially after subarachnoid hemorrhage (SAH). The aim is a closer investigation if rheology may help for better understanding of circulation disorders of CSF in the body.

The field of rheology can be divided in two types macro and micro rheology, according to different measuring setup. Macrorheology applies force on the sample to measure the deformation and on the other side for the passive microrheological analysis tracer particles are used which are driven by thermal energy (Brownian motion) which cause only minimal deformation to the estimated sample.

The samples were drawn via an external ventricular drainage at different time points after the SAH. Rheological measurements were operated with a rotational rheometer (Anton Paar Ltd., Graz, Austria) equipped with a double gap geometry (DG26,7/T200/SS). Different conditions in

the human body were simulated by measuring the samples at specific temperatures (5°C, 35°C, 37°C, 40°C), as the storage temperature in refrigerator – undercooled – physiologic – elevated body temperature. The frequency tests show a natural trend due to the different measuring temperatures. This specific data behavior was investigated further. Moreover, new methodology was used to calculate viscoelastic based parameters as the cumulative storage factor, which was introduced in previous works. These parameters were correlated with laboratory parameters, as erythrocyte and leukocyte count, total protein, lactate and glucose concentration.

Additionally, to the macrorheological characterization also microrheological analysis were operated with a Zetasizer Nano (Malvern Panalytical Ltd., Malvern, United Kingdom).

Relationships between the correlation of rheological and laboratory parameters and specific disease patterns of patients as well on the time elapsed since subarachnoid hemorrhage were observed. The overall goal is to evaluate whether rheological parameters have a clinical advantage and may help prediction of shunt dependence after SAH.

#### Acknowledgement

We would like to express our gratitude for the financial support provided by Impetus, Faculty of Medicine at Johannes Kepler University Linz, project number: MP0116101001 and LIT Institute of Technology at Johannes Kepler University Linz, project number: Ll113490001.

# OS7: Bioprocess Optimization for Succinic acid Production with an Engineered *Escherichia Coli* Strain Cultivated on Hydrolysates Derived from Municipal Solid Waste

**Petropoulos Apostolos**<sup>1</sup>, Margioulas Christos<sup>1</sup>, Ladakis Dimitrios<sup>2</sup>, Stylianou Eleni<sup>1</sup>, Koutinas Apostolis<sup>1</sup>

- <sup>1</sup> University of Athens, Department of Food Science and Human Nutrition, Iera Odos 75, 11885, Athens, Greece, Email: petropoulos.a95@gmail.com
- <sup>2</sup> National and Kapodistrian University of Athens, Department of Agriculture Development, Agri-Food and Natural Resources Management, Evripos Campus, 34400, Psachna, Evia, Greece

Keywords: Succinic acid, Escherichia coli, Municipal solid waste, Bioprocess optimization

The utilisation of renewable resources for the production of bio-based products is essential in order to develop sustainable bioprocesses. In the European Union, approximately 250 million t of municipal solid waste (MSW) are generated annually, with 86 million t constituting bio-waste (OFMSW). The disposal of biowaste in landfills significantly contributes to the release of greenhouse gas emissions. This is estimated to account for roughly 3% of European greenhouse gas emissions. [1] OFMSW has been evaluated as a potential feedstock for various bio-based products producing through fermentation processes, [2] including succinic acid (SA). SA is a vital platform chemical with numerous applications as a precursor for various derivatives. [3]

In this context, the present study assesses the production of SA using OFMSW hydrolysate. The bacterial strain *E. coli* AFP184 is employed in a two-stage cultivation process, with a primary focus on optimizing the fermentation process to enhance SA production.

The OFMSW can be considered as a promising feedstock for the biotechnological production of bio-based SA. The main components of OFMSW stream are free sugars (18.1%), glucan (14.7%), protein (9.8%) and starch (8.0%). The oil and pectin content of the OFMSW used in this study were 7.1% and 2.5%, respectively. Preliminary experiments were performed in Duran bottle fermentations in order to verify the ability of *E. coli* AFP184 to grow on commercial carbon sources that are contained in MSW hydrolysates. *E. coli* AFP184 did not consume sucrose and arabinose, and among the carbon sources tested, xylose and fructose exhibited the lowest efficiency. Galactose proved to be the most efficiently consumed

carbon source, reaching a concentration of 25.4 g/L, followed by mannose and glucose.

The optimization of the fermentation process was implemented in a bench-top bioreactor through fed-batch fermentations, involving the evaluation of various neutralizing agents (NaOH, KOH, NH<sub>4</sub>OH, Mg(OH)<sub>2</sub>) for pH regulation, the effect of volumetric oxygen transfer coefficient  $(k_{l}a)$  during aerobic phase and the initial carbon source concentration. Finaly, the optimum conditions were implemented on the biowaste fraction hydrolysates and were compared with glucose-rich synthetic medium in terms of final production, yield and productivity. When NaOH and KOH were used, no significant differences were observed in the overall fermentation efficiency. However, when NH<sub>4</sub>OH was employed, SA production reached 45.7 g/L, with a yield of 0.58 g/g and a productivity of 0.88 g/(L·h). Different  $k_l a$  values were evaluated (225.2-428.7 h<sup>-</sup> <sup>1</sup>) during aerobic phase. Among the  $k_{l}a$  values used the highest productivity (1.72 g/L/h) was observed at 388.0 h<sup>-1</sup> where cell growth was 17.4 g/L and succinic acid concentration was 34.6 g/L. Increasing the agitation rate to 1000 rpm (428.7  $h^{-1}$ ) resulted in lower biomass concentration (15.4 g/L), while succinic acid concentration reached 43.5 g/L. The effectiveness of the neutralizing agent,  $k_{L}a$  and initial carbon source concentration was evaluated using crude OFMSW hydrolysate as fermentation feedstock in fed-batch bioreactor fermentation. The main carbon source in the hydrolysate was glucose (about 86%), and SA production increased by approximately 15%.

The OFMSW can be considered a promising feedstock for the biotechnological production of bio-based SA.

#### References

- [1] *Biowaste in Europe turning challenges into opportunities*. A. Van der Linden, A. Reichel (Eds.), European Environment Agency, Kopenhagen, Denmark, 2020, p. 56.
- [2] M. Temirbekova, W. Wójcik, V. V. Stoyak, Journal of Ecological Engineering 22 (2021).
- [3] Z. Shu, H. Qin, B. Wu, F. Tan, J. Wang, M. He, Chin J App Environ Biol 21 (2015).10-21.

## Acknowledgement

The project is supported by the Circular Bio-based Europe Joint Undertaking and its members, funded by EU. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or CBE JU. Neither the European Union nor the CBE JU can be held responsible for them. This work was also co-funded by UK Research and Innovation (UKRI) under the UK government's Horizon Europe funding guarantee grant number 10082169.

# OS8: From Lignocellulosic Biomasses to Advanced Biopolymers in Just One Step

Mesto Davide<sup>1</sup>, Blasi Davide<sup>1</sup>, Tedeschi Vincenzo<sup>1</sup>, Coutgno Pietro<sup>1</sup>, Farinola Gianluca Maria<sup>1</sup>

<sup>1</sup> Università degli Studi di Bari "Aldo Moro", Dipartimento di Chimica, 70126, Email: davide.mesto@uniba.it and gianlucamaria.farinola@uniba.it

Keywords: lignin, lignin-first, lignocellulosic biomasses, ball miller, microwave-assisted extraction, one-pot functionalization, ethanosolv, pistachio shells

Developing economically sustainable processes for lignin valorization remains a significant challenge. Recently, a new paradigm known as "lignin-first" has emerged, focusing on lignin fractionation through biopolymer solvolysis followed by reductive stabilization to prevent biopolymer condensation.<sup>[1]</sup> Our research centers on ethanosolv processes aimed at achieving high retention of  $\beta$ -O-4 linkages in lignin fractions, using endocarps as feedstocks. Particularly, pistachio dried shells have shown promising results.<sup>[2]</sup> By optimizing biomass pre-treatment and utilizing microwave-assisted extraction, we achieved a delignification yield exceeding 70%, with lignin fractions primarily composed of S units and retaining approximately 70% β-O-4 linkages. However, the process duration, requiring 10 hours at 80°C, is a drawback. To enhance economic sustainability, we explored a single-step process that simultaneously extracts and functionalizes lignin. This approach eliminates the need for post-processing and enables

lignin functionalization with various species such as redox-active species such as gallic acid<sup>[3]</sup>, chromophores as rhodamine B, or antioxidants like ascorbic acid<sup>[4]</sup>, thus streamlining the process and reducing costs. The extraction-functionalization process exploits the acid environment of the extraction mixture to perform a microwave-assisted transesterification reaction between the carboxylic

acid group present on the additive molecular structure and the hydroxylic groups presents on lignin structure (Figure 1).



Figure 1: Gallic acid functionalization mechanism trough acid catalyzed transesterification

Our findings demonstrate that using pistachio shells as feedstock in an optimized ethanosolv process can yield high-quality lignin fractions with significant retention of  $\beta$ -O-4 linkages. While the process duration remains a challenge, the development of a single-step extraction and functionalization method offers a promising path toward more economically viable lignin valorization, transforming lignin from a waste to a versatile material. This integrated approach not only simplifies the process but also adds value to lignin by enabling its functionalization for various applications, potentially leading to broader industrial adoption and enhanced sustainability in biomass utilization.

## References

- [1] T. I. Korányi, B. Fridrich, A. Pineda, K. Barta, Molecules 25 (2020) 2815.
- [2] D. Blasi, D. Mesto, P. Cotugno, C. D. Calvano, M. Lo Presti, G. M. Farinola, Green Chem. Lett. Rev. 15 (2022) 893.
- [3] X. Shi, K. Wang, S. Gao, D. Zhang, C. Lai, C. Jin, M. Li, C. Wang, Q. Yong, F. Chu, *I&EC* 62, 43 (2023) 17765.
- [4] Y. Sheng, X. Tan, Y. Gu, X. Zhou, M. Tu, Y. Xu, Renew. Energy 163 (2021) 732.

## Acknowledgement

DB gratefully acknowledges the REFIN (Return for Future Innovation) action for funding, an initiative co-funded by European Union through the POR Puglia 2014–2020 (ID grant 2455F798). DM gratefully acknowledges the PON-RI Industrial Chemical and Molecular Sciences PhD XXXVII cycle action for funding, an initiative co-founded by European Union through the PON 2022–2025 for Green and Innovation topics (ID grant 634338).
## OS9: Aging of PE Hysteresis Loops of Hybrid-Doped PTC Ceramics

### Kryštof Koller<sup>1</sup>, Petr Ptáček<sup>1</sup>

<sup>1</sup> Brno University of Technology, Faculty of Chemistry, Institute of Materials Chemistry; Purkyňova 464/118, 612 00 Brno, Czech Republic; Email: krystof.koller@vut.cz

### Keywords: PTCR, BaTiO<sub>3</sub>, PE hysteresis loop, aging

BaTiO<sub>3</sub>, known for its robustness and structural simplicity, revolutionized ferroelectric ceramics. It was the first material used in manufacturing dielectric multilayer ceramic capacitors (MLCs). Doped with donors and acceptors, barium titanate finds applications in Positive Temperature Coefficient of Resistance (PTCR) ceramics, including self-regulating heaters, inrush current limiters, and SMD sensors [1,2].

Over time, ferroelectrics experience gradual degradation due to aging. While the exact microscopic processes behind aging are still debated, stable charged particles (such as oxygen vacancies  $V_0^{\bullet\bullet}$ ) are generally believed to play a main role. Aging is less pronounced in

highly pure materials or soft compositions but becomes more noticeable in hard compositions with acceptor dopants [3].

Our aged PE hysteresis loops show an increase in coercive field  $E_c$  and a decrease in spontaneous polarization  $P_s$  with time. Aging of ferroelectrics, based on this experiment and our previous measurement regarding aging of room temperature resistance ( $R_{25}$ ), can be explained by the volume effect with the symmetry-conforming principle, as proposed by Zhang and Ren [4].

### References

- [1] A. K. Bain, P. Chand, "Principles and Applications", in Ferroelectrics, Wiley-VCH Verlag GmbH & Co., 2017, p. 195.
- [2] M. Park, S. Kim, *Energies* 10 (2017) 10.
- [3] V. Koval, G. Viola, Y. Tan, "Biasing Effects in Ferroic Materials", Ferroelectric Materials Synthesis and Characterization, Jul. 2015.
- [4] L. Zhang, X. Ren, Physical Review B 70 (2006) 9.

### Acknowledgement

This work was supported by TDK Electronics s.r.o.

# OS10: Bismuth and Antimony Halide Perovskites – Progress and Potential Practical Application of Environmentally Friendly Hybrid Semiconductors

**Stevan Gavranovic**<sup>1</sup>, Salvatore Valastro<sup>2</sup>, Ioannis Deretzis<sup>2</sup>, Emanuele Smecca<sup>2</sup>, Jan Pospisil<sup>1</sup>, Oldrich Zmeskal<sup>1</sup>, Antonino La Magna<sup>2</sup>, Martin Vala<sup>1</sup>, Alessandra Alberti<sup>2</sup> and Giovanni Mannino<sup>2</sup>

- <sup>1</sup> Brno University of Technology, Faculty of Chemistry, Materials Research Centre, Purkynova 118, 612 00 Brno, Czech Republic, Email: Stevan.Gavranovic@vut.cz
- <sup>2</sup> National Research Council (CNR), Institute of Microelectronics and Microsystems (IMM), Strada VIII n°5 Zona Industriale, 95121 Catania, Italy

Keywords: optoelectronics, photovoltaics, lead-free, halide perovskites, detectors

Lead halide perovskite (LHP) materials have attracted a lot of attention due to their unique optoelectronic properties: high absorption coefficients, long charge carrier diffusion lengths, low defects density, and tunable bandgap. Owing to their brilliant properties, they have been explored as many different optoelectronic devices, such as solar cells, photodetectors, LEDs, memristors, etc. Solar cells based on LHP have achieved a steep increase in power conversion efficiency over the years, from 3.9 % (2009) to over 26 % (2023). Commonly studied halide perovskites have the general formula of ABX<sub>3</sub>, where A is a monovalent cation methylammonium (CH<sub>3</sub>NH<sub>3</sub><sup>+</sup> or MA<sup>+</sup>), formamidinium (CH(NH<sub>2</sub>)<sub>2</sub><sup>+</sup> or FA<sup>+</sup>) or cesium (Cs<sup>+</sup>); B is a bivalent cation lead (Pb<sup>2+</sup>) or tin (Sn<sup>2+</sup>); and X is a halide anion chloride (Cl<sup>-</sup>), bromide (Br<sup>-</sup>) or iodide (l<sup>-</sup>). However, the presence of lead (II) cations in the structure of HPs has raised concerns about the environmental impact and waste management of future perovskite devices.

Thus, there is a persistent challenge to substitute the lead in the structure of halide perovskites while maintaining the desired optoelectronic properties. The most obvious substitution with  $Sb^{2+}$  leads to instability and structural changes due to the oxidation of  $Sb^{2+}$  to  $Sb^{4+}$ .

One of the most perspective substitutional strategies is the heterovalent substitution where two Pb<sup>2+</sup> ions are substituted with one monovalent cation (typically MA<sup>+</sup> or Cs<sup>+</sup>) and one trivalent cation (bismuth Bi<sup>3+</sup> or antimony Sb<sup>3+</sup>). This substitution leads to the formation of very stable perovskite structures A<sub>3</sub>Bi<sub>2</sub>X<sub>9</sub>. Nevertheless, due to the low dimensionality of their crystalline lattices, they have complex and less efficient charge transport.

In this contribution, we present the preparation of monocrystalline and polycrystalline forms of two lead-free perovskites, methylammonium bismuth iodide ( $MA_3Bi_2I_9$ ) and methylammonium antimony iodide ( $MA_3Bi_2I_9$ ).

The prepared samples were the subjects of an advanced structural and optical characterization, which was later used to discuss the possible practical application of these lead-free perovskites. In fact, the analysis of the absorption coefficients shows a significant difference between the two studied materials. In MA<sub>3</sub>Bi<sub>2</sub>I<sub>9</sub>, we notice a clear excitonic peak at an energy of 2.49 eV, while the MA<sub>3</sub>Sb<sub>2</sub>I<sub>9</sub> samples have no presence of the excitonic peak.



Figure 1: a) device based on single crystals; b) device based on polycrystalline thin films

To explore the application potential of these materials, we fabricated two sets of devices. The devices based on monocrystalline perovskites consisted of the active material sandwiched between carbon electrodes, as shown in Figure 1a. The polycrystalline devices were fabricated by drop coating technique using the Solaronix® monolithic perovskite solar cell architecture presented in Figure 1b.These devices were later studied under visible light (1sun illumination) and under X-ray radiation. Both devices have shown an extremely low dark current (below 1 nA) and an evident increase in charge current densities after irradiation. This contribution compares the energy conversion between the two different device architectures and the two different materials MA<sub>3</sub>Bi<sub>2</sub>I<sub>9</sub> and MA<sub>3</sub>Sb<sub>2</sub>I<sub>9</sub>. The most favorable practical application is proposed based on the output performance of the studied devices.

### References

- [1] M. Cheng, J. Jiang, C. Yan, Y. Lin, M. Mortazavi, A.B. Kaul, Q. Jiang, Nanomaterials 14 (2024) 5.
- [2] S. Valastro, S. Gavranovic, I. Deretzis, M. Vala, E. Smecca, A. La Magna, A. Alberti, K. Castkova, G. Mannino, Advanced Optical Materials 12 (2024) 11.

### Acknowledgement

The authors acknowledge the financial support from JCMM Brno Ph.D. Talent, the Interfaculty project FCH/FSI-J-24-8521 and FCH-S-24-8592, and the SAMOTHRACE project (ECS00000022, CUP B63C22000620005).

# PW1: Search for Poly-Hydroxyalkanoates Producers in the Microbiota from Hypersaline Environments

Adhvaryu Shivani<sup>1</sup>, Malinicova Lenka<sup>1</sup>, Piknova Maria<sup>1</sup>, Pristas Peter<sup>1</sup>

<sup>1</sup> Department of Microbiology, Institute of Biology and Ecology, Faculty of Science, Pavol Jozef Šafárik University in Košice, Šrobárova 2, 04154 Košice, Slovakia, Email: shivani.adhvaryu@student.upjs.sk

### Keywords: Halophiles, Halotolerant, Archaebacteria, Polyhydroxyalkanoate (PHA)

Prokaryotes in extreme environments gained researchers' attention as they could be used in various biotechnological and commercial applications [1]. Poly-hydroxyalkanoates (PHAs) are one of the possible biomolecules that have the potential to replace the fossil fuel dependency of mankind and enhance sustainable and eco-friendly bioplastic production [2]. Many microorganisms produce under stressful conditions PHAs as inclusion bodies, which act as a storage compound [3]. Recent studies have identified halophilic prokaryotes as a promising source of PHAs.

In our experiments, PHA production was analyzed in prokaryotes from several naturel hypersaline environments (see Table 1). Water samples were inoculated on R2A, TSA and CMH media with 5%, 10% and 15% of NaCl and the bacteria obtained were further characterized.

MALDI-TOF mass spectroscopy was used for the initial dereplication, and a representative of each MALDI group was selected for the 16S rRNA gene sequence-based identification. To detect PHA production MM (Minimal media) plates with few modifications was used [3]. The isolates were stained using Nile Blue and PHAs production was observed as orange fluorescence under UV light [4].

Table 1: The occurrence of PHA positive isolates in tested hypersaline environments

In all tested environments, multiple halophilic isolates were detected and further characterized. More than 100 halotolerant or halophilic heterotrophic isolates were obtained and characterized. The bacterial colonies showing bright orange fluorescence under UV light were scored PHA-positive. Table 1 summarizes the data on PHApositive strains from three different localities.

No significant effect of isolation medium or NaCl concentration used on cultivable microbiota diversity in the Solivar, Presov was observed. The sampling season had the most important impact on observed diversity. The Shannon diversity index values for the years 2020, 2021, and 2022 are 1.896, 1.861, and 3.783, resp. The low diverse halophilic microbiota represented bv Proteobacteria members (mainly Chromohalobacter and Halomonas spp.) observed in 2020 and 2021 was replaced by more diverse population of halotolerant gram-positive bacilli (mainly Halobacillus, Rossellomorea, Priestia, Peribacillus, and Bacillus spp.) observed in 2022. In natural salt spring Slana voda in Oravska Polhora Proteobacteria genus Halomonas was found to be dominant. The eubacterial isolates were widely positive for PHAs production in both Solivar and Oravska Polhora sampling sites. All the archaeal species isolated from the Pomorie, Bulgaria salt pan showed no evidence of PHAs production.

Sampling		Number of Strains		Dominant PHA positive	
Locality	Source	Time	Tested	PHA positive	genus
Solivar, Slovakia	Salt brine	Sept 2020	22	21	Chromohalobacter
		Sept 2021	15	10	Halomonas
		May 2022	53	11	Halobacillus
Oravska Polhora, Slovakia	Salt spring	May 2022	12	12	Halomonas
Pomorie, Bulgaria	Salt pan	Nov 2023	30	0	Halorubrum

### References

[1] B. Dutta, R. Bandopadhyay, Beni-Suef University Journal of Basic and Applied Sciences 11 (2022) 75.

[2] G.Y. Tan, C.L. Chen, L. Li, L. Ge, L. Wang, I.M.N. Razaad, Y. Li, L. Zhao, Y. Mo, J.Y. Wang, Polymers 6 (2014) 706-754.

[3] E. Quesada, A. Ventosa, F. Rodriguez-Valera, L. Megias, A. Ramos-Cormenzana, *Microbiology* 129 (1983) 2649-2657.

[4] S. Obruča, P. Dvořák, P. Sedláček, M. Koller, K. Sedlář, I. Pernicová, D. Šafránek, *Biotechnology Advances* 58 (2022) 107906.

### Acknowledgement

This work was supported by VVGS-PF-2023-2545 grant from Pavol Jozef Safarik University in Kosice and VEGA-1/0779/21 grant.

# PW2: Interesting Metabolism of Polyhydroxyalkanoate Production in the "Hot" Genus Aneurinibacillus

**Buchtíková Iva**<sup>1</sup>, Řeháková Veronika<sup>1,2</sup>, Šlosárová Katarína<sup>1,2</sup>, Dvořáková Dominka<sup>1</sup>, Obruča Stanislav<sup>1,2</sup>

- <sup>1</sup> Faculty of Chemistry, Brno University of Technology, Institute of Food Chemistry and Biotechnology, Purkyňova 464/118 61200 Brno, Email: xcpernicovai@fch.vut.cz
- <sup>2</sup> Materials Research Centre, Faculty of Chemistry, Brno University of Technology, Brno, Czech Republic

### Keywords: thermophiles, polyhydroxyalkanoates, Aneurinibacillus, copolymers

Polyhydroxyalkanoates (PHA) are very interesting and promising materials microbial polyester which are produced by many various bacteria. Additionally, there are completely biodegradable and biocompatible, providing a wide range of end uses. PHA can also be produced from renewable sources, making them a suitable alternative to plastics made from petroleum. However, production is expensive. Fortunately, PHA are also produced by extremophiles, on which the next generation of biotechnological production is based [1]. Extremophilic organisms live in extreme conditions and due to this fact, the biotechnological process is not so demanding on sterility and the cost of production is lowery.

Using our original isolation protocol [2], thermophilic bacteria of the genus *Aneurinibacillus* were isolated from

activated sludge and compost. This genus proved to be a suitable candidate to produce polyhydroxyalkanoates. These bacteria are able to produce not only homopolymers composed only of 3-hydroxybutyrate (3HB) units, but also interesting copolymers which, in addition to the 3HB monomer, contain 4hydroxybutyrate [3] or other very unusual monomers such as 3-hydroxyvalerate, 4-hydroxyvalerate or 5hydroxyvalerate [4]. The composition of the copolymer depends on the medium used and also on the precursor. Also, their metabolism of PHA synthesis differs from that of conventional PHA producers. PHA production also occurs in complex media where there is no nitrogen limitation. One of the strains was deposited as a patent culture in the Czech collection of microorganisms.

### References

- [1] G. Q. Chen, X.R. Jiang, Current Opinion in Biotechnology 50 (2018) 94-100
- [2] I. Pernicova et al., International Journal of Biological Macromolecules 144 (2020) 698-704.
- [3] I. Pernicova et al., Polymers 12 (2020) 1235.
- [4] V. Rehakova et al., International Journal of Biological Macromolecules 225 (2023) 1588-1598.

# PW3: Microbial Cultivation: *Cupriavidus Necator* DSM 545 and *Hydrogenophaga Pseudoflava* DSM 1034 in Prosecco Wine Lees

Caminiti Viola<sup>1</sup>, Favaro Lorenzo<sup>1,2</sup>, Casella Sergio<sup>1</sup>, Basaglia Marina<sup>1</sup>

- <sup>1</sup> University of Padova, Department of Agronomy, Animals, Food, Natural resources and the Environment, Viale dell'Università, 16, 35020 Legnaro, Italy, Email: viola.caminiti@phd.unipd.it
- <sup>2</sup> University of Stellenbosch, Department of Microbiology, Private Bag X1, Matieland 7602, South Africa

Keywords: Prosecco wine lees; Polyhydroxyalkanoates; *Cupriavidus necator; Hydrogenophaga pseudoflava*; Bioplastic; Circular economy.

Nowadays, in the agricultural and agro-industrial sectors, there is increasing attention on the wine industry. Italy leads European countries in wine production, manufacturing approximately 47.5 million hectoliters (MhI) annually making it the top nation globally, followed by France, with 42.1 MhI, and Spain, with 33.5 MhI. The environmental impact of wine production, particularly in terms of waste generation, is a growing concern. On average, per each hectoliter of wine produced, about 196 L of wastewater, 0.1 kg of sludge (dry matter) and 1.6 kg of wine lees are generated [1].

Wine lees is a sludge material that forms at the bottom of wine tanks after alcoholic fermentation which low pH, high content of organic matter and phenolic compounds and high discharge temperature. In the production of sparkling wines, the must undergoes multiple fermentation, resulting in the availability of wine lees, commonly referred to as fine lees, throughout the year. Despite their usage for biogas production and extraction of compounds, such as antioxidants, tartaric acid and ethanol [2], their potential in bioplastic production, specifically polyhydroxyalkanoates (PHAs), remains largely untapped. These biopolymers have gained much attention as a promising substitute for petroleum-based plastics due to their higher biodegradability and biocompatibility properties. Unfortunately, the realization of cost-effective large-scale production for PHAs necessitates a mandatory reduction in manufacturing costs [3].

This study aims to evaluate the potential use of wine lees as a medium sustaining bacterial growth and PHAs accumulation. Specifically, *Cupriavidus necator* DSM 545 and *Hydrogenophaga pseudoflava* DSM 1035, were cultivated in the liquid phase of wine lees obtained from the Prosecco winemaking. *C. necator* DSM 545 accumulated 42.90% of cell dry weight (CDW) and 1.27 g/L of PHAs when grown on pure distilled wine lees. *H. pseudoflava* DSM 1035, on the same substrate, reached values of 1.60 g/L and 40.42% CDW of PHAs.

### References

- [1] C. Da Ros, C. Cavinato, P. Pavan, D. Bolzonella. Journal Waste Management 34 (2014) 2028–35
- [2] A. De Iseppi, M. Marangon, S. Vincenzi, G. Lomolino, A. Curioni, & B. Divol. Lwt 136 (2021) 110274.
- [3] L. Favaro, M. Basaglia, S. Casella, *Biofuels, Bioproducts and Biorefining* 13(1) (2019) 208-227.

### Acknowledgement

This work was supported by the University of Padova [Grant number BIRD234877/23; 2024; DAFNAE1DOR-00156, DOR2352129; DOR2297411/22; DOR2107797/21]. V.C. was a recipient of a doctoral scholarship from the University of Padova.

# PW4: PHA-Related Regulatory Small RNAs in *Caldimonas Thermodepolymerans*

Heřmánková Kristýna<sup>1</sup>, Xenie Kouřilová<sup>2</sup>, Iva Buchtíková<sup>2</sup>, Stanislav Obruča<sup>2</sup>, Sedlář Karel<sup>1</sup>

- <sup>1</sup> Brno University of Technology, Department of Biomedical Engineering FEEC, Technická 3058/10,
  616 00 Brno-Královo Pole, Email: 211200@vut.cz
- <sup>2</sup> Brno University of Technology, Department of Food Chemistry and Biotechnology, Faculty of Chemistry, Purkynova 464/118, 612 00, Brno

Keywords: *Caldimonas thermodepolymerans*, small RNA, RNA-Seq, transcriptome, polyhydroxyalkanoates

Small RNAs represent a group of post-transcriptional regulatory elements, a part of the machinery regulating gene expression in bacteria. These non-coding regulatory elements are not translated into proteins, and therefore can act as rapid responses to stress. The sRNA molecule is after transcription able to bind an mRNA target, and by multiple mechanisms determine whether to discard the mRNA or not. With this principle, levels of mRNAs in cells are influenced in response to changing environments and the needs of bacteria.

Caldimonas thermodepolymerans DSM 15344<sup>T</sup> is a moderately thermophilic bacterium, a promising candidate for application in biotechnology. This bacterium is primarily known for the production of polyhydroxyalkanoate (PHA) granules, a source material for bioplastics. C. thermodepolymerans also represents a candidate for the Next generation industrial biotechnology (NGIB) [1] approach that aims for sustainable production using bacteria. The NGIB tries to reduce the biotechnological production costs by finding bacterial candidates that are able for efficient production without the need for expensive conditions for batch production [1]. To further investigate the capacity of C. thermodepolymerans metabolism, we used the transcriptomic data measured with RNA-Seq to infer sRNAs and conduct downstream analyses.

The drawback of the sRNAs analyses is the lack of their structural annotations in bacterial genomes and thus they need to be first predicted. One option represents the prediction of sRNAs from RNA-Seq data as the transcription from intergenic regions.

As well as the structural annotation, the functional annotation of sRNAs is missing. Therefore, to find putative small RNAs that relate to PHA metabolism, we conducted a co-expression analysis to infer the functionality of sRNAs with a 'guilt by association' approach. These sRNAs that have similar expression profiles to those genes known to be involved in PHA

### References

- [1] Chen, G. Q., & Jiang, X. R. Current Opinion in Biotechnology, 50, 94–100 (2018).
- [2] Musilova, J. et al., Computational and Structural Biotechnology Journal, 21 (2023).

### Acknowledgement

This work has been supported by grant project GACR 22-10845S.

metabolism [2] were further investigated. The numbers of all sRNAs predicted in *C. thermodepolymerans'* genome are shown in *Table 1*, as well as the number of sRNAs probably involved in PHA metabolism.

Table 1: Inferred sRNAs in C. thermodepolymerans' genome.

small RNAs	all sRNAs	PHA metabolism related
trans	5	4
cis	731	259

The candidate sRNAs were predicted from RNA-Seq samples measured from the cultivation of bacterium with xylose. Three biological replicates were measured in 8 time points to cover 72 hours. The growth graph with the production of PHB is shown in *Figure 1*.



Figure 1: Growth and PHB production of C. thermodepolymerans DSM 15344<sup>T</sup>.

With the help of state-of-the-art tools, further analyses lead to the structural and functional annotation of sRNAs. Using a 'guilt by association' approach, those sRNAs that were assigned to genes involved in PHA metabolism were further investigated.

These results provide deeper insight into the sRNAs regulatory mechanism of *C. thermodepolymerans* DSM 15344<sup>T</sup>. Overall, results contribute to the assessment of bacterial utilization in industrial applications by providing further knowledge of bacterial capacity.

# PW5: The Promise of Caldimonas Thermodepolymerans in Sustainable Production of Polyhydroxyalkanoates

Kouřilová Xenie<sup>1</sup>, Buchtíková Iva<sup>1</sup>, Musilová Jana<sup>2</sup>, Sedlář Karel<sup>2</sup>, Dvořák Pavel<sup>3</sup>, Obruča Stanislav<sup>1</sup>

- <sup>1</sup> Faculty of Chemistry, Brno University of Technology, Purkyňova 464/118, Brno, 612 00, Czechia, Email: xckourilovax@fch.vut.cz
- <sup>2</sup> Faculty of Electrical Engineering and Communication, Brno University of Technology, Technická 3082/12, Brno, 616 00, Czechia
- <sup>3</sup> Faculty of Science, Masaryk University, Kamenice 5, Brno, 625 00, Czechia

### Keywords: NGIB, polyhydroxyalkanoates, thermophiles, Caldimonas, Tepidimonas, Rubrobacter

The overuse and improper disposal of petrochemical plastics is a significant global environmental issue. A potential solution lies in polyhydroxyalkanoates (PHA), biodegradable and biocompatible biopolymers that can substitute for certain commercial plastics. However, the production costs of PHA are still higher than those of petroleum-based plastics. To address this, strategies such as utilizing extremophilic bacteria and waste materials as substrates have been proposed, aligning with the 'Next Generation Industrial Biotechnology' concept [1]. Extremophiles, a diverse group of microorganisms, hold considerable potential for biotechnological applications. Thermophilic bacteria, in particular, offer advantages like reduced environmental sterility requirements, higher substrate solubility, and decreased cooling water needs.

Some thermophiles also produce PHA as intracellular inclusions for carbon and energy storage.

Caldimonas thermodepolymerans (basionym Schlegelella thermodepolymerans), a thermophilic bacterium, stands out as a promising PHA producer. This species uniquely utilizes xylose, favoring it over other substrates such as glucose [2]. Xylose, the second most abundant carbohydrate on earth, is found in lignocellulosic materials, which are major waste sources. Leveraging xylose as a carbon source opens numerous possibilities for sustainable PHA production. This research delves into the sugar metabolism of *C. thermodepolymerans* and its link to PHA synthesis, emphasizing its potential as a viable candidate for cost-effective PHA production under the Next Generation Industrial Biotechnology framework.

### References

[1] G. Q. Chen, X. R. Jiang, Current Opinion in Biotechnology (2018) 50.

[2] X. Kourilova et al., *Bioresource Technology* (2020) 315.

### Acknowledgement

This study was funded by the project GA22-10845S of the Czech Science Foundation (GACR).

# PW6: Pretreatment of Sawdust Using Deep Eutectic Solvent for Poly(3-hydroxybutyrate) (PHB) Production

Margioulas Christos<sup>1</sup>, Feith Maëlys<sup>2</sup>, Filippi Katiana<sup>1</sup>, Psaki Olga<sup>1</sup>, Koutinas Apostolis<sup>1</sup>

- <sup>1</sup> Department of Food Science and Human Nutrition, Agricultural University of Athens, Athens, Greece. Email: chris.margioulas@gmail.com
- <sup>2</sup> Department of Biology, Polytech Clermont-Ferrand, Clermont-Ferrand, France.

Keywords: Sawdust, Deep Eutectic Solvent, Lignocellulosic biomass, Enzymatic hydrolysis, Poly(3-hydroxybutyrate)

The present study demonstrates the development of a bioprocess for the efficient bioconversion of sawdust into poly(3-hydroxybutyrate) (PHB). Sawdust is a readily available and abundant byproduct of industrial and agricultural activities which poses significant challenges in terms of effective utilisation and proper waste management. The recalcitrant structure of sawdust, due to its lignocellulosic nature, is the main obstacle impeding the efficient saccharification of polysaccharides. Therefore, a pretreatment step, in order to disrupt the complex structure of lignocellulosic biomass and remove lignin, is essential to enhance the efficiency of enzymes in hydrolyzing cellulose and hemicellulose.

Owing to the growing interest in replacing the currently used chemical solvents for biomass pretreatment, Deep Eutectic Solvents (DES) were used in this study. DES are eutectic mixtures composed of a hydrogen bond acceptor (HBA) and a hydrogen bond donor (HBD). Compared to traditional solvents, DES exhibit more environmentally friendly behavior when released into the environment [1].

In this study, DES were prepared by mixing choline chloride (ChCl) as HBA and lactic acid (LA) as the HBD in a molar ratio of 1:10. Initially, sawdust was pretreated with DES using a Parr reactor system at six distinct temperatures (100°C, 120°C, 140°C, 160°C, 180°C and 200°C) and different pretreatment durations (30 to 120 min). Sawdust was suspended in the solvent as a solid loading of 10%. The pretreated biomass was recovered by filtration and washed with distilled water until it reached neutral pH.

Enzymatic hydrolysis of the pretreated biomass was performed by utilizing commercial enzyme preparations containing cellulase,  $\beta$ -glucosidase, xylanase, and glucoamylase. All hydrolysis experiments were conducted at 50°C for 48 h with a 1:10 solid-to-deionised water ratio under mechanical stirring. In all cases, the pH of the hydrolysis was adjusted to 5.0.

The hydrolysate produced after the enzymatic hydrolysis of pretreated sawdust was used as carbon source for PHB production with the bacterial strain *Paraburkholderia sacchari* DSM 17165. The fermentation was carried out under phosphorus limitation in order to trigger the polymer accumulation, while the bioreactor conditions were based on Psaki et al. [2].

Sawdust used in this study is mainly composed of cellulose (43.2%), xylose (10.0%), galactose (1.9%), mannose (9.5%) and lignin (27.2%). After the pretreatment, the lignin removal achieved was more than 36%. By utilizing the pretreated solids as a substrate for enzymatic hydrolysis, more than 64.8% glucan-to-glucose conversion yield was achieved. The total sugars in the hydrolysate were over 46 g/L. Finally, the hydrolysate produced under optimal pretreatment conditions was used as a carbon source for biopolymer production in bioreactor cultures. The fed-batch fermentation resulted in the production of 100 g/L total dry weight with PHB content higher than 50% (w/v).

These findings underscore the effectiveness of DES in enhancing sawdust valorisation and highlight the potential of sawdust as a sustainable feedstock for value-added products. The study demonstrates a viable method for the conversion of sawdust into valuable biochemical products and also contributes to the broader goals of waste reduction and sustainable resources utilization.

### References

[1] K. Filippi, E. Stylianou, C. Pateraki, A, Koutinas, D. Ladakis, *Waste and Biomass Valorization* 14 (2023), 2857-2872.
 [2] O. Psaki, I. G. I. Athanasoulia, A. Giannoulis, D. Briassoulis, A. Koutinas, D. Ladakis, *Bioresource Technology* 382 (2023), 129077.

# PW7: Process Simulation and Techno-Economic Evaluation of Various Polyhydroxyalkanoates (PHA) Production Processes

Ozturk Abdullah Bilal<sup>1,2</sup>, Xenie Kourilova<sup>2</sup>, Obruča Stanislav<sup>2</sup>

- <sup>1</sup> Department of Chemical Engineering, Faculty of Chemical and Metallurgical Engineering, Yildiz Technical University, Esenler, Istanbul 34220, Türkiye, Email: bozturk@yildiz.edu.tr
- <sup>2</sup> Department of Food Chemistry and Biotechnology, Faculty of Chemistry, Brno University of Technology, Purkynova 118, 612 00 Brno, Czech Republic

Keywords: polyhydroxyalkanoates, process simulation, techno-economic assessment, *Halomonas halophila*, *Caldimonas thermodepolymerans* 

Polyhydroxyalkanoate (PHA) is a well-known family of bacteria-based biodegradable plastics that offer an approach to carbon neutrality and contribute to a more sustainable future. PHAs are a crucial platform chemical and can serve as an environmentally friendly candidate for replacing petrochemical plastics [1]. It can be used in several industries, including bioplastics, the medical and pharmaceutical industry, textile and fibers, and agriculture. Some bacteria, such as Halomonas halophila and Caldimonas thermodepolymerans can produce PHAs from a wide range of carbon sources such as lignocellulosic biomass, food waste, and sugar sources, and similar to other biotechnological processes, several challenges affect the feasibility and marketability of the PHAs [2]. Scale-up difficulties, strain development for high PHAs production capabilities, energy-intensive downstream, and yield could be considered significant challenges for a feasible process. Therefore, process simulation and comprehensive economic evaluation are promising approaches for potential industrial-scale production. In this study, softwood and rice straws were used as lignocellulosic substrates and converted into PHA via halophilic and thermophilic conditions. The key parameters and data for the economic evaluation and process simulation were obtained from experimental studies and available literature. The industrial-scale PHA production scenarios were prepared with these data using SuperPro Designer software v11.0 (Intelligen Inc., Scotch Plains, NJ, USA). The project lifetime was set at 20 years with an 8000-h working time per year [3-4]. The flowsheets for the industrial-scale PHAs production process were prepared to process 50,000 tons of lignocellulosic biomass annually [5]. As a result, these two processes were comprehensively evaluated regarding process bottlenecks, the economic burden of the plant, and saving strategies, including by-product utilization and virtual heat integration. The results clarified that halophilic PHA production from soft-wood was a more economically favorable option compared to thermophilic PHA production from rice straw due to higher NPV (213.2 million \$), IRR (13.5%), ROI (16.4%), GM (62.4%), and shorter PBP (5.07 years).

### References

- Novackova, I., Kourilova, X., Mrazova, K., Sedlacek, P., Kalina, M., Krzyzanek, V., Koller, M., Obruca, S., *Polymers* 14 (2022) 1761.
- [2] Kourilova, X., Novackova, I., Koller, M., Obruca, S., Bioresource Technology 325 (2021) 124704.
- [3] Ozturk, A.B., Arasoglu, T., Gulen, J., Cheng, S., Al-Shorgani, N.K.N., Habaki, H., Egashira, R., Kalil, M.S., Yusoff, W.M.W., Cross, J.S., Sustainable Energy & Fuels 5 (2021) 3705–3718.
- [4] Gutiérrez Ortiz, F.J., Journal of Supercritical Fluids 160, (2020) 104788.
- [5] Teghammar, A., Forgács, G., Sárvári Horváth, I., Taherzadeh, M.J., Applied Energy 116 (2014) 125–133.

# PW8: Thermophilic Bacteria of the *Aneurinibacillus* Genus: Producers of Unique α-Methylated PHA Copolymers

Řeháková Veronika<sup>1</sup>, Pernicová Iva<sup>1</sup>, Petr Sedláček<sup>2</sup>, Michal Kalina<sup>2</sup> and Stanislav Obruča<sup>1</sup>

- <sup>1</sup> Brno University of Technology, Faculty of Chemistry, Institute of Food Science and Biotechnology, Purkyňova 464/118, 61200 Brno, Email: xcrehakovav@vutbr.cz
- <sup>2</sup> Brno University of Technology, Faculty of Chemistry, Institute of Physical and Applied Chemistry, Purkyňova 464/118, 61200 Brno

### Keywords: polyhydroxyalkanoates, copolymers, thermophilic bacteria, Aneurinibacillus

Polyhydroxyalkanoates (PHA) are valuable biopolymers primarily synthesized by bacteria, serving as their carbon and energy source. Apart from being biocompatible, biodegradable, and non-toxic, PHAs share similarities with conventional plastics derived from petrochemical sources. However, the most commonly produced PHA, poly(3-hydroxybutyrate) (P(3HB)), often lacks sufficient elasticity, making it stiff and brittle. Introducing structurally diverse PHA monomers into its composition effectively reduces overall crystallinity, thereby enhancing elasticity and resulting in the PHA polymer being more suitable for various applications.



Figure 1: PHA granules within aneurinibacilli cells.

Recently, thermophilic gram-positive bacteria of the Aneurinibacillus genus emerged as promising candidates for producing diverse PHA copolymers. In addition to common monomers like 3-hydroxybutyrate and 3hydroxyvalerate, they have demonstrated biosynthesis capabilities for 4-hydroxyvalerate, 4-hydroxyhexanoate, 4hydroxybutyrate, and 5-hydroxyvalerate [1,2]. To push their limits further, we explored the utilization of  $\alpha$ methyl-y-butyrolactone, a precursor for biosynthesizing  $\alpha$ branched copolymers - an uncommon class of PHA polymers. Thermophilic bacteria of the Aneurinibacillus genus successfully biosynthesized poly(3HB-co-4-hydroxy-2-methylbutyrate) up to 11.14 mol% of total PHA content. GC-FID and NMR analyses confirmed the presence of the desired copolymer. Subsequently, we conducted experiments varying PHA additional precursor concentrations (lactone and glucose) and analyzed resulting materials using SEC-MALS, DSC, and FTIR, revealing distinctive properties. This marks the first evidence of wild-type bacteria producing (P(3HB-co-4H2MB)).

Thermophilic *Aneurinibacillus* bacteria represent a unique bacterial species with a rare ability to produce diverse PHA copolymers. This trait is likely due to their highly versatile PHA synthases, making bacteria of the genus *Aneurinibacillus* an intriguing candidate for genetic engineering in other species.

### References

- [1] I. Pernicova, I. Novackova, P. Sedlacek et al., Polymers (2020), 12(6) 1235.
- [2] V. Rehakova, I. Pernicova, X. Kourilova et al., Int. Jour. of Biol. Macromol. (2023), 225, 1588-1598.

### Acknowledgement

This study was funded by the junior project FCH/FEKT-J-24-8516.

### PW9: Conversion of Ferulic Acid by Extremophilic Bacteria

**Vendula Hrabalová**<sup>1</sup>, Tomáš Opial<sup>1</sup>, Jana Musilová<sup>2</sup>, Karel Sedlář<sup>2</sup>, Jaromír Pořízka<sup>1</sup>, Pavel Diviš<sup>1</sup>, Stanislav Obruča<sup>1</sup>

- <sup>1</sup> Department of Food Chemistry and Biotechnology, Faculty of Chemistry, Brno University of Technology, Purkyňova 118, 612 00 Brno, Czech Republic, Email: Vendula.Hrabalova@vut.cz
- <sup>2</sup> Department of Biomedical Engineering, Faculty of Electrical Engineering and Communication, Brno University of Technology, Technická 12, 616 00 Brno, Czech Republic

### Keywords: Thermophiles; halophiles, ferulic acid; biotransformation; vanillic acid; vanillyl alcohol

Biotransformation of ferulic acid (FA) involves the metabolic activities of microorganisms such as bacteria or fungi, which alter the chemical structure of compounds. FA, a phenolic compound prevalent in numerous plants, offers a multitude of health benefits including anti-cancer, anti-inflammatory, and antioxidant effects. This compound can be efficiently sourced from lignocellulosic waste, which is abundant in agricultural and forestry byproducts.

Through microbial biotransformation, FA can be converted into several valuable products, such as vanillic acid, vanillyl alcohol, vanillin, and 4-vinylguaiacol. These biotransformed products find applications in various industries, particularly in pharmaceuticals, food, and cosmetics, due to their beneficial properties. For instance, vanillin is widely used as a flavoring agent, while vanillic acid and vanillyl alcohol are used in the synthesis of complex molecules for drug development.

Extremophilic bacteria were used in this work. These bacteria can survive in environments with extreme conditions such as high/low temperature, acidic or basic environments, or high salt concentration. Their ability to survive in conditions that are unfavorable to other microorganisms reduces the risk of contamination and therefore the cost of producing the desired substances.

The use of extremophilic bacteria in the biotransformation of FA is an innovative approach that holds significant potential for creating new therapeutic compounds. Extremophilic bacteria, which thrive in extreme environmental conditions, possess unique metabolic pathways that can be harnessed for efficient biotransformation processes. This experiment specifically employed a thermophilic bacterium, *Caldimonas* 

thermodepolymerans, known for its ability to function at high temperatures and halophilic bacteria strain *Halomonas neptunia*, which thrive in salt environment of concentration 81 g/L.



# Figure 1: The process of performing the ferulic acid biotransformation experiment

The experiment was carried out in flasks, where ferulic acid was added to the culture medium (complex/production) at different concentrations. During cultivation in the production medium, not only ferulic acid was converted but also polyhydroxyalkanoates (PHAs) were produced. PHAs are polyesters that are accumulated by microorganisms in the form of intracellular granules and have similar properties to synthetic plastics. Biotransformation experiments have achieved a conversion success rate of 80–90 mol. %.

### Acknowledgement

This study was funded by the projects GA22-10845S (GACR) and by FW02020135 (TACR).

# PW10: Production of Microbial Pigments by Selected Members of Genus Massilia

Kollerova Silvia<sup>1</sup>, Bockova Sabina<sup>1</sup>, Benesova Marketa<sup>2</sup>, Obruca Stanislav<sup>1</sup>

- <sup>1</sup> Brno University of Technology, Faculty of Chemistry, Institute of Food Science and Biotechnology, Purkynova 464/118, 612 00 Brno, Czech Republic, Email: silvia.kollerova@vut.cz
  - <sup>2</sup> Institute of Scientific Instruments, Czech Academy of Sciences, Královopolská 147, 612 64, Brno, Czech Republic

### Keywords: microbial pigments, extremophiles, Raman spectroscopy

Color is essential for many consumer products that are a day-to-day part of our lives. Even though synthetic colorants currently dominate the markets, consumers demand safe and natural alternatives that also have a lower environmental impact than the conventional ones currently used. Microbial pigments have favorable characteristics and potentially broad areas of application with advantages over the conventional pigments such as biodegradability and low toxicity. Moreover, microbial pigments offer added benefits that are valuable for various industries, such as antioxidative, antimicrobial, or antitumor properties [1, 2, 3]. The combination of these factors makes them very interesting for developing replacements for conventional colorants and dyes. It is therefore important to identify producers of microbial pigments that can potentially be developed into highly productive cell factories and to study the pigments produced by these bacteria, as novel properties can be discovered.

The bacteria belonging to a genus *Massilia* reside in many different environments, from areas with cold temperatures, such as Antarctica to warmer areas such as Mexico. Members of this group can be found in soil and air samples, as well as in biofilm on the surface of rocks. While some members of this genus are known to produce pigments, some strains have also been reported for their ability to produce polyhydroxyalkanoates (PHAs) [4].

This study evaluated pigments produced by selected members of *Massilia* genus. Several of the selected strains are psychrophiles that were sampled from Antarctica. The selected bacterial strains have not been yet very well studied and the available data on their pigment production are scarce.

Ten selected bacterial strains of *Massilia* genus were cultivated from lyophilizates. The produced pigments were analyzed by Raman spectroscopy. To analyze samples for any content of PHA, Fourier-transform infrared spectroscopy (FTIR) was utilized. Subsequently, multiplex PCR and gel electrophoresis were used to confirm or exclude presence of PHA synthase in five *Massilia* strains that were selected for their strong pigmentation.

Our results suggest that the selected members of *Massilia* genus produced several types of pigments, some of the bacteria were also able to co-produce PHA. The presence of PHA synthase was also confirmed in some of the strains. These results suggest that some of the selected members of *Massilia* genus can potentially be utilized as cell factories for the co-production of industrially interesting pigments and PHA.

### References

- [1] E. Milosevic, N. Stanisavljevic, S. Boskovic et al., J Cancer Res Clin Oncol 149 (2023) 10975–10987.
- [2] H. Im, S.Y. Choi, S. Son et al., Sci Rep 7 (2017) 14415.
- [3] R.K. Suryawanshi C.D. Patil, J.M. Ames et al., J Virol 94 (2020).
- [4] D. Jeon, L. Jiang, K. H. Kim, et al., *Sci Rep* 13 (2023) 17767.

# PW11: Characterization of Topography and Mechanical Properties of Bacterial Cells

Markéta Khýrová<sup>1, 3</sup>, Eva Slaninová<sup>1</sup>, Petr Sedláček<sup>1</sup>, Josef Šepitka<sup>2</sup>, Vojtěch Černý<sup>2</sup>, Tomáš Plichta<sup>3</sup>

- <sup>1</sup> Faculty of Chemistry, Brno University of Technology, Purkynova 118, Brno, 612 00, Czech Republic, Email: Marketa.Khyrova@vut.cz
- Faculty of Mechanical Engineering, Czech Technical University in Prague, Technicka 4, Prague 6, 166 07, Czech Republic
- <sup>3</sup> Institute of Scientific Instruments, Czech Academy of Sciences, Kralovopolska 147, Brno, 612 00, Czech Republic

### Keywords: atomic force microscopy, nanoindentation, bacteria, polyhydroxyalkanoates

Recently, there has been increased interest in the mechanical properties of prokaryotic microorganisms such as bacteria. For this purpose, two of the bacterial strains *Cupriavidus necator* and *Rhodospirillum rubrum* which possess unique ability to accumulate intracellular substances called polyhydroxyalkanoates or shortly PHAs, that act as an energy storage for the cells [1]. The aim is to understand these bacteria as deeply as possible in order to increase the production but at the same time reduce the production costs for PHAs, which are biodegradable and biocompatible polymers with the potential applications in many different fields.

The cells were selected in PHA-producing variant along with the non-producing mutant from both strains. Measurements were carried out using atomic force microscope (AFM) and nanoindenter in liquid phosphate buffer medium to ensure the physiological conditions. Bacterial cells had to be immobilized on a glass substrate using poly-L-lysine to perform the experiments.



Figure 1: AFM image of Rhodospirillum rubrum (PHAproducing)

References

- [1] T. Narancic, E. Scollica, G. Cagney a K. E. O'Connor. Microbiology 164(2018) 4, 625-634..
- [2] JPK INSTRUMENTS. JPK NanoWizard AFM Handbook: JPK NanoWizard AFM Handbook. Online. Nanotechnology for Life Science. Version 6.0. Berlin: JPK BioAFM Center, 2018.
- [3] A. Overbeck, S. Günther, I. Kampen a A. Kwade. Chemical Engineering and Technology 40 (2017) 6, 1158-1164.

AFM measurements were performed in the liquid environment using JPK NanoWizard 4 microscope in QI<sup>TM</sup> mode. For this purpose, MLCT – A or MLCT-SPH-1UM-DC – A probes on cantilevers with the spring constant around 0,1 N·m<sup>-1</sup> were used. In this way, topographic maps of these cells were obtained. The force-distance curves were also evaluated to determine the elastic modulus of the cells using Hertzian contact analysis [2].

Nanoindentation measurements were also carried out in the liquid environment using Hysitron BioSoft instrument in the displacement control mode. The constant loading rate of diamond flat punch tips (R<sub>c</sub> 20 and 50  $\mu$ m) was 10  $\mu$ m·s<sup>-1</sup>. This way the single-cell microcompression tests were performed in which the single analyzed cell was compressed until its complete rupture. The obtained curves were then evaluated according to the modified Overbeck model [3] and the elastic modulus was determined.

AFM and microcompression analyses revealed significant topographical and mechanical differences between PHA-producing and non-producing bacteria which exhibit different values of elastic modulus. While AFM revealed much lower values of elastic modulus (averaging from hundreds to thousands of kPa), nanoindentation would give average values 10× higher. In addition, the results from both methods revealed that the PHA-producing bacteria exhibited higher elastic modulus values on average than their non-producing mutant.

## PW12: Cultivation of Carotenogenic Yeasts on Complex Waste Substrates from the Food Industry under Combined Stress

**Obračaj Jan**<sup>1</sup>, Holub Jiří<sup>1</sup>, Špačková Dominika<sup>1</sup>, Baťková Zuzana<sup>1</sup>, Šnejdrlová Kateřina<sup>1</sup>, Gerspitzerová Nela<sup>1</sup>, Márová Ivana<sup>1</sup>

 <sup>1</sup> Institute of Food Science and Biotechnology, Faculty of Chemistry, Brno University of technology, 612 00 Brno, Czech Republic, Email: Jan.Obracaj@vut.cz.

Keywords: red yeast, carotenoids, waste substrate, yeast biomass, fatty acids, bioreactors.

This research is focused on the biotechnology of carotenogenic yeasts. This type of microorganism is specific in producing many valuable metabolites, including carotenoid pigments, fatty acids, ubiquinone, ergosterol, beta-glucans and certain exopolysacharides. Many of these are powerful antioxidants, provitamins and have many other positive effects on human health when supplemented. This yeast biomass and metabolites are used for example in the pharmaceutical, cosmetic or food industry and therefore have great potential.

The biggest challenge in cultivating these microorganisms lies in their demand for nutritional sources of carbon, nitrogen and some microbiogenic elements, which is usually the most costly aspect of this activity. However this type of yeast is known for its ability to utilize many nutritional resources, including various waste substrates. This fact gives us space for the application of the so-called circular economy.

The food industry waste substrates selected for this work include brewery spent grain hydrolysate, yeast extracts prepared from sedimented brewer's yeast and waste whey from the dairy industry. The research work also includes investigating the pretreatment of these substrates to create the most suitable environment for the cultivation of the biomass under study and for their highest possible yield.

The effect of addition of different amounts of selected microbiogenic elements on yeast biomass production was also investigated using whey waste substrate. The research also included a brief analysis of selected exopolysaccharides (EPS) produced by these microorganisms during cultivation.

Metabolites contained in final biomass, were analyzed by various laboratory techniques, including gas chromatography (GC), high performance liquid chromatography (HPLC), fluorescence microscopy etc.

The results obtained in this work suggest that treated brewer's spent grain and yeast extract prepared from brewer's spent yeast are suitable for the cultivation of carotenogenic yeasts and can also serve as a source of total nitrogen nutrient during cultivation. For the utilization of whey substrate under the influence of combined stress, the best results are shown for the strain *Cystofilobasidium macerans*.



*Figure 1: Microscopic display of strain Rhodotorula toruloides (magnify 100x).* 

The results of this work can provide valuable informations with application in industrial biotechnology of carotenogenic yeasts and can provide economically interesting use of selected industrial wastes.

# PW13: Effect of Adaptation to Continuous Osmotic Stress on the Bacterium Rhodospirillum Rubrum

Pacasova Viktorie-Alexandra<sup>1</sup>, Fiala Tomas<sup>2</sup>, Eva Slaninova<sup>2</sup>, Stanislav Obruca<sup>2</sup>

- <sup>1</sup> Department of Food Chemistry and Biotechnology, Faculty of Chemistry, Brno University of Technology, Purkynova 464/118 Brno 612 00, email: Viktorie-Alexandra@vutbr.cz
- <sup>2</sup> Department of Food Chemistry and Biotechnology, Faculty of Chemistry, Brno University of Technology

Keywords: *Rhodospirillum rubrum*, osmotic stress, polyhydroxyalkanoates, evolutionary engineering, gas chromatography, flow cytometry

In recent years, there have been major advances in industry which, in addition to improving the quality of everyday life, has also caused massive enviromental pollution (e.g. plastic pollution). This issue could be solved by replacing the petrochemical plastics by in nature biodegrable materials such as polyhydroxyalkanoates (PHAs) also produced by purple non-sulfur bacterium *Rhodospirillum rubrum*. The advantage of this bacterium as a PHA producer is its metabolic versatility and thus its ability to survive in various conditions (light, dark, anaerobic or aerobic conditions, etc.) [1, 2]. This work focused on the adaptation of *R. rubrum* to osmotic stress by evolutionary engineering with the goal of increased PHA production.

First, the bacterial strain was exposed to different salt concentrations in order to optimize the appropriate salt concentration for subsequent adaptation experiment. During the evolutionary experiments, the PHA content of the adapted strains was analyzed by GC-FID, and the total dry biomass was also determined. After the evolutionary experiments, the cultures were exposed to selected stressors (high temperature; osmotic shock and freezing-thawing cycles) followed by viability analysis of by flow cytometry. In the last experiment, a comparison was made between the adapted and wild-type strains, where both strains were cultivated in media with different carbon sources (respectively acetate or fructose). The medias also contained different salt concentrations (0, 40 and 60 g/l NaCl). After culturing, the PHA content was determined by GC-FID.

We were able to confirm the positive effect of continuous exposure to osmotic stress of 40 g/l NaCl on PHA production in R. rubrum with the concentration of 15–20 % throughout the The method experiment. of evolutionary engineering seems to be appropriate for increasing PHA production in *R. rubrum*. In the future, it would be worthwhile to extend this work by including adaptations to other stressors in combination with carbon substrates other than those used in this work.

### References

[1] T.D. Brock, M.T. Madigan, J.M. Martinko, J.Parker, *Biology of Microorganisms*, Upper Saddle River: Prentice Hall, 2000, p. 459.

[2] G. Cohen-Bazire, R. Kunisawa, Journal Of Cell Biology. 1963, p. 401-419.

### Acknowledgement

This work was supported by project GA 21-15958L of Czech Science Foundation.

# PW14: Biohydrogen - the Fuel of the Future, or the Study of Hydrogen Production by *Clostridium Butyricum* and *Clostridium Tyrobutyricum*

Pacasova Viktorie-Alexandra<sup>1,4</sup>, Matej Poulicek<sup>2</sup>, Josef Stetina<sup>2</sup>, Stanislav Obruca<sup>3</sup>

- <sup>1</sup> Department of Food Chemistry and Biotechnology, Faculty of Chemistry, Brno University of Technology, Purkynova 464/118 Brno, 612 00, email: Viktorie-Alexandra@vutbr.cz
- <sup>2</sup> Institute of Automotive and Transport Engineering, Faculty of Mechanical Engineering, Brno University of Technology
- <sup>3</sup> Department of Food Chemistry and Biotechnology, Faculty of Chemistry, Brno University of Technology
- <sup>4</sup> Materials Research Centre, Faculty of Chemistry, Brno University of Technology

Keywords: *Clostridium butyricum*, *Clostridium tyrobutyricum*, anaerobic bacteria, biohydrogen, alternative fuel, sustainable energy

With the rapid development of industry and its deepening impact on climate change, interest in the possible use of alternative energy sources has been growing in recent years. Much of this interest is focused on electricity from natural renewable energy sources (solar energy, hydroelectric or wind power, etc.). Another suitable type of renewable energy is the production of combustible gases such as methane or hydrogen. The downside of methane, however, is that its combustion produces CO<sub>2</sub>, which also contributes to already increasing greenhouse gas emissions. In contrast, when burning hydrogen, which is a clean, efficient and fully recyclable energy source, only water vapour is produced [1].

A solution to this problem could be the biotechnological production of hydrogen using microorganisms capable of producing it using carbohydrate-rich waste materials from the food industry. Among the promising hydrogen producers are bacteria of the genus *Clostridium*. These bacteria, which are strict anaerobes, produce hydrogen through two metabolic pathways, namely acetic and butyric fermentation, using organic matter as the primary source of hydrogen and energy. These organic substrates include glucose and other hexoses, lactose, sucrose, starch, etc [2].

This work focuses on the description of hydrogen production by the anaerobic bacteria *Clostrodium butyricum* and *Clostridium tyrobutyricum* with a focus on the optimal conditions for biohydrogen production such as culture time, suitable medium, temperature, pH, etc. Furthermore, his work focuses on the development of a suitable apparatus for the collection of the produced gas mixture followed by the analysis of the composition of produced gas mixture by Hiden QGA ("quantitative gas analysis"), based on the quadrupole principle, which is used for continuous analysis of gases and vapours.

### References

[1] D. Liu, *Bio-hydrogen production by dark fermentation from organic wastes and residues*. DTU Environment Technical University of Denmark, Miljoevej, 2008, p. 60

[2] H. Argun, F. Kargi, I.K. Kapdan, International Journal of Hydrogen Energy, p. 34

### Acknowledgement

This work was supported by project BD162403001 of Brno University of Technology

# PW15: Transcriptomic Analysis of *Rhodospirillum Rubrum* Wild-Type and Mutant Strains

**Sabatova Katerina**<sup>1</sup>, Jakubickova Marketa<sup>1</sup>, Slaninova Eva<sup>2</sup>, Fleuriot-Blitman Hugo<sup>3</sup>, Amstutz Véronique<sup>3</sup>, Kristyna Hermankova<sup>1</sup>, Zinn Manfred<sup>3</sup>, Obruca Stanislav<sup>2</sup>, Sedlar Karel<sup>1</sup>

- <sup>1</sup> Department of Biomedical Engineering, Faculty of Electrical Engineering and Communication, Brno University of Technology, Technicka 3082/12, 616 00 Brno, Czechia, Email: sabatovak@vut.cz
- <sup>2</sup> Department of Food Chemistry and Biotechnology, Faculty of Chemistry, Brno University of Technology, Brno, Czechia
- <sup>3</sup> Institute of Life Technologies, University of Applied Sciences and Arts Western Switzerland Valais-Wallis (HES-SO Valais-Wallis), Sion, Switzerland

### Keywords: Rhodospirillum rubrum, RNA-Seq, gene ontology

*Rhodospirillum rubrum* is a versatile bacterium capable of thriving under various cultivation conditions, including both aerobic and anaerobic environments. It is also known as a promising candidate for production of biopolymers such as polyhydroxyalkanoates (PHA), which are of significant interest for biodegradable plastic production. However, comprehensive genome-wide transcriptomic studies are lacking, limiting our ability to fully explore gene regulation in *R. rubrum*, particularly in relation to PHA production.

In our study, we present an analysis of RNA-Seq data of *Rhodospirillum rubrum* DSM  $467^{T}$  wild-type strain and *ΔphaC1ΔphaC2* mutant strain [1]. Both strains were cultivated under identical conditions using either fructose or acetate as a substrate, with RNA samples collected at the same grow phases.

The resulting RNA-Seq data were analyzed to uncover the main differences between the cultivation conditions and between the two strains on transcriptomic level. To achieve this, we employed differential expression analysis and gene ontology (GO) enrichment analysis to identify GO terms associated with the most significant changes in gene expression under the studied conditions.

The results were visualized as show in Figure 1, where a heatmap represents the expression profiles of selected genes associated with significantly enriched GO terms, and arrows indicate statistically significant changes in the gene expression. For instance, Figure 1 compares of cultivations of *R. rubrum* wild-type strain on fructose and acetate, highlighting enriched GO terms such as electron transfer activity (molecular function (MF) GO term) and response to stress (biological process (BP) GO term).

Our analysis provides further insights into the responses of *R. rubrum* wild-type and  $\Delta phaC1\Delta phaC2$ 

mutant strains to specific substrates, enhancing our understanding of their metabolic adaptability and potential for biopolymer production.



Figure 1: Expression profiles of selected genes of wild-type R. rubrum cultivated with either fructose or acetate. Heatmap shows z-scores calculated from average gene expression. Arrows represent results from differential expression analysis:  $\supseteq$  down regulation,  $\nearrow$  up regulation at p adj value < 0.05, B.-H. correction.

### References

[1] K. Jureckova, M. Nykrynova, E. Slaninova, et. al., *Computational and Structural Biotechnology Journal* 23 (2024) 2681-2694.

### Acknowledgement

This study was supported by the bilateral grant project GACR 21-15958L / SNSF 205321L\_197275/1.

# PW16: Nobody is Perfect – Genetic Modification of Thermophilic Bacteria

Šlosárová Katarína<sup>1</sup>, Buchtíková Iva<sup>1</sup>, Sedlář Karel<sup>2</sup>, Dvořák Pavel<sup>3</sup> and Obruča Stanislav<sup>1</sup>

- <sup>1</sup> Dpt. of Food Chemistry and Biotechnology, Faculty of Chemistry, Brno University of Technology, Brno, Czechia, Katarina.Slosarova@vut.cz
- <sup>2</sup> Dpt. of Biomedical Engineering, Faculty of Electrical Engineering and Communication, Brno University of Technology, Brno, Czechia
- <sup>3</sup> Dpt. of Experimental Biology, Section of Microbiology, Masaryk University, Brno, Czechia

Keywords: thermophilic bacteria, polyhydroxyalkanoates, genetic modification

GMOs or genetically modified organisms have been a major topic of debate in recent years. Even though some people believe they are dangerous, all myths have been dispelled and, in addition to improving the properties of the organism itself, they have been shown to help the environment in more ways than simply providing nutrition for more people – reducing excess  $CO_2$ , using fewer chemicals and fuels during the farming process, preventing soil erosion improving soil health, and saving water. GMOs also include micro-organisms, which are mainly used in biomedical applications. We propose a combination of genetic modification of bacteria to help the environment, but this time directly linked to a major environmental problem of our time – plastic pollution.

Closely related to this issue are the bacteria's own metabolites – polyhydroxyalkanoates (PHA). These intracellularly produced granules have attracted particular attention due to their properties similar to petrochemical plastics and the attributes of being biobased, non-toxic, and biodegradable. Apart from the aforementioned sphere, their use is particularly promising in the field of biomedicine (biocontrol agents, drug carriers, biodegradable implants, tissue engineering, memory enhancers, and anticancer agents).

Our two hot candidates are thermophilic bacteria of the genus *Aneurinibacillus*, which have recently been identified by our group as significant producers of unique PHA copolymers revealing extraordinary material properties, and *Caldimonas thermodepolymerans*, a moderately thermophilic bacteria that is capable of

### Acknowledgement

This work is supported from the grant Brno Ph.D. Talent

accumulating a significant amount of poly3hydroxybutyrate P(3HB) from lignocellulose relevant sugars. However, *Aneurinibacilli* are extremely sensitive to even small modifications when cultivated and they also form endospores, P(3HB) itself as a homopolymer does not excel in industrial applications. Since no one is perfect, our vision is to connect these two (already) great worlds into one "Simply the best".

Table 1: Potential strategies to improve PHA production
involving gene deletion in addition to gene transfer

Gene and organisms	Modification	The aim of the modification
phaC and phaR from Aneurinibacillus sp.	Transfer into C. thermodepolymeras	Establish synthesis or unique PHA copolymers in C. thermodepolymerans
Colum Genes encoding for intracellular depolymerases ( <i>phaZi</i> ) in both bacteria	Deletion of the genes	Column Enhancing both PHA yields and also molecular weight of the polymers
Genes involved in endotoxin synthesis in C. thermodepolymerans	Deletion of the genes	Elimination of the endotoxins (the most problematic impurities of PHA) concerning their use in medical applications

# PW17: Study of Methylomes in *Aneurinibacillus* Species using Third Generation Sequencing Platform

**Umair Mohammad**<sup>1</sup>, Rehakova Veronika<sup>2</sup>, Bezdicek Matej<sup>3</sup>, Buchtikova Iva<sup>2</sup>, Obruca Stanislav<sup>2</sup>, Sedlar Karel<sup>1</sup>

- <sup>1</sup> Department of Biomedical Engineering, Faculty of Electrical Engineering and Communication, Brno University of Technology, Technická 3058/10, 61600 Brno-Kralove Pole, Mohd.Umair@vut.cz
- <sup>2</sup> Department of Food Chemistry and Biotechnology, Faculty of Chemistry, BUT
- <sup>3</sup> Department of Internal Medicine Hematology and Oncology, University Hospital Brno

Keywords: methylation, Aneurinibacillus, Oxford Nanopore, bacterial genomics.

Detection of methylation in bacterial genomes has been crucial in understanding how gene regulation, pathogenesis and adaptation work in bacteria [1]. It helps us understand how genetic and metabolic capabilities can help us understand the industrial potential of the bacteria. Thermophilic members of the *Aneurinibacillus* genus are gram-positive spore-forming bacteria species recently identified as producers of polyhydroxyalkanoates (PHAs) [2], a precursor for bioplastics. In this study, we utilized Oxford Nanopore Technologies (ONT) sequencing to investigate methylomes in *Aneurinibacillus* sp. AFN2 across various genomic features.

Sequencing was done using the PromethION system with R10.4 flow cells. Genomic annotation was conducted using the Prokka tool [3], for comprehensive gene prediction and functional annotation. The sequences were basecalled using the modified basecalling feature of Dorado, later Modkit was employed to handle modified bases from ONT, specifically for converting modBAM to bedMethyl files using best practices.

The sequence analysis showed us the significant number of modifications being present in the *Aneurinibacillus* bacterial genome as seen in Table 1.

Table 1: Modification	Counts Summary
-----------------------	----------------

	Modification	Count	
1	6mA	31022	
2	5mC	24040	

Out of the Total modifications, 50,808 were found to be in the coding region (CDS) out of which 22,003 were 5mC and 28,805 were 6mA modifications which is around 92% of the total of the total modifications. In the rRNA region, 1,526 5mC sites and 1,534 6mA modification sites were detected while in repeated regions 48 5mC sites and 54 6mA sites, highlighting their potential role in genome stability and regulation. tRNA showed 5 sites of 5mC and

### References

- [1] L.D. Moore, T. Le, G. Fan, Neuropsychopharmacology 38 (2013) 23-38.
- [2] Y. Subhash, H. J. Kim, S. S. Lee, International Journal of Syst Evol Microbiol 67 (2017), 2544-2548.
- [3] Seemann T. Prokka, Bioinformatics 30 (2014) 2068.

### Acknowledgement

This work was supported by Inter Faculty Junior Project 2024- FCH/FEKT-J-24-8516.

22 sites of 6mA modification as shown in Figure 1. The total of 1065 modifications were not found in any annotated feature.



Figure 1: Distribution of modifications across genomic features

Furthermore, we also calculated the modification density for both methylation types. The density of 5mC modification was found to be around 0.006 per base while the density of 6mA modification was approximately 0.008 per base thus indicating the higher occurrence of 6mA modification in the bacterial genome.

These findings determine the widespread methylation pattern and are distributed among various genomic features. Most of the methylation in CDS shows the role played by methylation in gene regulation and expression in the bacteria. The differential distribution of 5mC and 6mA across genomic features can provide insights into various functional roles and regulatory mechanisms within the genome. This study underscores the robustness of ONT sequencing in detecting and quantifying DNA methylation, offering valuable insights into the epigenetic landscape of *Aneurinibacillus* species.

# PW18: Hydrogel Bioinoculants: Enhancing Plant Resistance to Drought Stress

Černayová Diana<sup>1</sup>, Rousk Johannes<sup>2</sup>, Sedláček Petr<sup>1</sup>, Obruča Stanislav<sup>1</sup>

- <sup>1</sup> Faculty of Chemistry, Brno University of Technology, Purkyňova 464/118, Brno 612 00, Czechia, Email: xccernayova@vutbr.cz
- <sup>2</sup> Lund University, Box 117, Lund SE-221 00, Sweden

Keywords: Bioinoculants, Alginate, Hydrogels, PGPR

Climate change has a significant influence on an agricultural production worldwide. Watering of plants and crops is essential and desirable, nevertheless consistent high temperatures demand careful monitoring and optimization of irrigation practices to mitigate water loss and maintain crop yields. One potential solution for retaining water could be the implementation of hydrogels with encapsulated plant-growth promoting bacteria (PGPR).

Azotobacter *vinelandii* belongs to plant growth promoting rhizobacteria (PGPR) and shows biological activities for the stimulation of plant growth and is capable of synthesizing two completely different biopolymers with great application potential. Polyhydroxyalkanoates (PHA) are produced and stored in the form of intracellular granules improving cell robustness, while alginate is produced extracellularly and used for bacterial protection.

In this work, hydrogels with encapsulated bacteria, by direct gelation of bacterial alginate, are formed and employed into the soil with lettuce seeds. After 40 days of plant grow, we stopped watering the plants and observed how the plants were influenced by drought. The experiment showed positive results not only in the improved condition of plants (including higher biomass and increased content of both plants and roots), but also in higher resistance to drought in treated plants compared to untreated ones.



Figure 1 Schematic presentation of the experiment

### Acknowledgement

The research is supported by Czech Science Foundation number GA23-06757S.

# PW19: The Effect of Plant Growth-Promoting Rhizobacteria Application on Soil Properties and Growth of Model Plants in a Pot Cultivation Experiment

Kalina Michal<sup>1</sup>, Hlaváčková Barbora<sup>1</sup>, Súkeník Martin<sup>1</sup>, Sedláček Petr<sup>1</sup>

<sup>1</sup> Brno University of Technology, Faculty of Chemistry, Institute of Physical and Applied Chemistry, Purkyňova 464/118, Brno, Czech Republic, Email: kalina-m@fch.vut.cz

Keywords: alginate gel, PGPR, BIOLOG EcoPlate<sup>™</sup>, plant growth, pot cultivation

Plant Growth Promoting Rhizobacteria (PGPR) are soil bacteria, which presence in soil significantly influence soil properties and its fertility. Conventional ways of soil management connected with the application of inorganic fertilizers can have severe impact on soil physicochemical properties (soil organic matter stability, soil density and compactness, water holding capacity) and soil microbiological characteristics (soil microorganisms' quantity, variability and vitality). In recent time, there have been several tendencies to overcome this issue by environmentally friendly way. One of the promising possibilities how to improve soil properties and health is the application of soil conditioners, biostimulants and bioinoculants [1-4].

The main aim of the work was the optimization of the application form of PGPR (bacteria incorporated in alginate gel, freeze-dried gel with bacteria, bacterial suspension, alginate gel without bacteria, control sample). These different PGPR-formulations [1] were applied in soil and studied the effects on growth and vitality of model plants (*Lactusa sativa, Zea mays*) in a driven pot cultivation experiment (controlled automatic irrigation and illumination, measured temperature, moisture). Growth aspects of model plants were assessed online during the plant vegetation cycle (monitoring of plant height, width,

number of leaves) and after the termination of plant vegetation cycle (weights of fresh and dried plant, above and underground plant weight, roots density and vitality by using the image analysis tools). Beside the effect on plant growth we also assessed the effects of various application forms on PGPR on soil microbial activity by using the commercial BIOLOG EcoPlate<sup>TM</sup> kit and also the effects on soil physico-chemical properties (soil moisture, pH, organic and mineral content of soil).

The results of the work indicated that gel form with entrapped PGPR and freeze-dried gel with PGPR had the most significant effects on plant growth (highest weight of roots and plants) compared to the blank samples without PGPR application. The application of different PGPR forms did not have statistically significant effects on soil physicochemical properties, but on the other hand BIOLOG EcoPlate tests revealed the positive effects of gel form and freeze-dried gel form with entrapped PGPR bacteria application on soil microorganisms' activity.

The results of our work confirmed the positive effects of PGPR on soil microbiological and agronomical properties and verified our proposed concept of the preparation PGPR inoculants via entrapment of PGPR inside the alginate hydrogel.

### References

- [1] Z. Segaye, T. Alemu, F.A. Desta, F. Assefa, Frontiers in Microbiology 13 (2022) 1-9.
- [2] A. Rammenou, et el., Earth Systems and Environment 7 (2023), 583-600.
- [3] M. Kalina, et al., Agronomy 12 (2022), 1768.
- [4] S. Sovova, et al., Ecocycles 7 (2021) 46-54.

### Acknowledgement

The work was supported by the Czech Science Foundation of the Czech Republic (GACR project no. GA23-06757S).

## PW20: Slow-release Nitrogen Fertilizers with Biodegradable Poly(3hydroxybutyrate) Coating

### Krobot Štěpán<sup>1</sup>, Kontárová Soňa<sup>1</sup>, Přikryl Radek<sup>1</sup>

<sup>1</sup> Brno University of Technology, Faculty of Chemistry, Purkyňova 464/118, Brno, 612 00, Czech Republic; email: Stepan.Krobot@vut.cz

# Keywords: slow-release fertilizers, polyhydroxyalkanoates, poly(3-hydroxybutyrate), coating, nitrogen-based fertilizers

Fertilizers are crucial in meeting the increasing demand for food in agriculture. However, excessive concentrations and uncontrolled leaching of nutrients contribute to environmental pollution by increasing reactive, unassimilated nitrogen levels. This study explores the formulation and characteristics of slow-release fertilizers coated with fully biodegradable poly(3hydroxybutyrate), offering a gradual nitrogen release without soil pollution.

Urea, a nitrogen fertilizer, was pelletized and then coated with a solution of poly(3-hydroxybutyrate) in dioxolane, forming a thin, high-quality polymer coating. Testing revealed that some coated pellets retained excellent resistance even after 76 days submerged in water. Pot experiments conducted in Mitscherlich vegetation vessels assessed the impact of these coated fertilizers on maize growth and soil nitrogen release dynamics. Results demonstrated that utilizing these coated fertilizers effectively supplies maize plants with necessary nutrients while ensuring the poly(3hydroxybutyrate) coating does not impede maize growth. [1,2]

Our coated pellets containing 50% fertilizer with 50% P3HB showed excellent resistance and even after 76 days in water, only 20% of the urea content was released. According to a review of controlled-release fertilizers by Lawrencia et al. [3], such fertilizer release in the water environment corresponds more to fertilizer with a polymer-based coating than fertilizer with a natural polymer-based coating. We proved the feasibility of P3HB as a filler and coating material. By adjusting filler content and coating thickness, we could design the period of the

agrochemical release from the formulation. Effective P3HB coating could also be used for seed protection.

The pot experiment results proved coated fertilizers as a possible option to improve nutrient use efficiency, reduce nitrogen losses, and minimize environmental pollution while providing nitrogen to plants more gradually during vegetation,

Our research on controlled-release fertilizers with biodegradable coating involved coated formulations with urea and P3HB filler. We were able to prepare these pellets on a quarter-operational pelletizing device and coat them in larger quantities in a coating drum. This technology could be transferable to the industry. A careful study of the biodegradation of these fertilizer formulations in soil and research into the long-term effect on soil composition under field conditions will also be needed.



Figure 1: Tests of prepared P3HB coated slow-release fertilizers with maize

### References

[1] L.T. Fan, S.K. Singh, In *Controlled Release: A Quantitative Treatment*, L.T. Fan, S.K. Singh (Eds.), Springer Science & Business Media: Berlin/Heidelberg, Germany, 2012, p. 1–8.

[2] J.C. Cole, M.W. Smith, C.J. Penn, B.S. Cheary, K.J. Conaghan, Scientia Horticulturae 211 (2016) 420-430.

[3] D. Lawrencia, S. K. Wong, D.Y.S. Low, B.H. Goh, L.H. Lee, S.Y. Tang, Plants 10 (2021) 238.

### Acknowledgement

Authors acknowledge the funding by Brno University of Technology by the Specific University Research Grant through the project FCH-S-23-8208.

# PW21: Enhancing Soil Health: Hydrogel Self-Encapsulation of Azotobacter

**Súkeník Martin<sup>1</sup>**, Černayová Diana<sup>2</sup>, Kalina Michal<sup>1</sup>, Hlaváčková Barbora<sup>1</sup>, Sedláček Petr<sup>1</sup>, Obruča Stanislav<sup>2</sup>

- <sup>1</sup> Faculty of Chemistry Brno University of Technology, Institute of Physical and Applied Chemistry, Czech Republic, Email: Martin.Sukenik@vut.cz
- <sup>2</sup> Faculty of Chemistry Brno University of Technology, Institute of Food Science and Biotechnology, Czech Republic

### Keywords: Alginate, Azotobacter vinelandii, polyhydroxyalkanoates, PGPR

The increasing demands for sustainable agriculture require innovative approaches to achieve comparable yields with reduced use of conventional fertilisers, hence improving the environmental sustainability of agricultural practices and preventing irreversible damage to fertile land. Among these innovative technologies belongs development of biofertilizers that inoculate soil with plant growth-promoting rhizobacteria (PGPR), the wide group of microbes known for their beneficial effects such as nitrogen fixation, phosphate dissolution, siderophore and phytohormone production [1], and the synthesis of protective exopolysaccharide alginate and intracellular polyhydroxyalkanoates serving as a carbon source under stress conditions [2].

The research introduces a novel concept of biofertilizer production using well-known PGPR Azotobacter vinelandii for in-situ self-encapsulation in gel carrier via crosslinking of the alginate produced during culturing of the bacterium. This concept simplifies the preparation procedure with the possibility of reducing costs and increasing the competitiveness of the whole process. The validation of this concept involved subjecting selected strains to gelation experiments under alginate gel formation using a 2 wt. % CaCl<sub>2</sub> cross-linking agent. Azotobacter vinelandii strains DSM 87, DSM 720, DMS 85, DSM 13529, DSM 576, and CCM 289 were chosen for the preparation and characterisation of bioinoculants. Among these, Azotobacter Vinelandii CCM 289 was preferred due to its high alginate production, effective gelation ability, and confirmed capacity to produce indole-3-acetic acid and siderophores.

A pilot cultivation experiment was conducted on a model plant (*Lactuca sativa*) with the addition of different PGPR carrier compositions, where each application form was marked with the appropriate colour (Table 1), and each application form or group contained 8 plants (in total of 40). During the whole cultivation experiment, drought stress was induced in the plants by low irrigation and therefore soil moisture in the range of 12.2-24.0 %. After 29 days, the basic parameters of the plants in the form of fresh weight, dry weight, as well as leaf length, root length, chlorophyll a, chlorophyll b, and carotenoid content were analysed.

Table 1: Overview of the different PGPR carrier

compositions

Colour group	Carrier composition of PGPR
Red	Cells in PBS
Yellow	Gel without cells
Green	Gel with cells
Blue	Freeze-dried gel with cells
White	Negative control (without any addition)

All data are presented as relative values with respect to the negative control, defined as 100 %. All groups of plants treated with the PGPR carrier composition showed significantly higher values of fresh and dry weights compared to the negative control, and the yellow group showed the highest increase in fresh and dry weights at 3293±989 and 1353±282 %, respectively. The highest leaf length was also observed in the yellow group, reaching 325±19 %. The most significant increase in root length was recorded in the blue group by  $174\pm28$  %. The chlorophyll a and chlorophyll b values were highest in the green group by  $110\pm24$  % and  $156\pm43$  %, respectively. The negative control contained the highest carotenoid content, in the treated cultures, the relative content ranged between  $46\pm18$  % (red group) and  $100\pm51$  % (white group).

### References

- [1] A. Hasan, B. Tabassum, M. Hashim, N. Khan, Bacteria 3 (2024) 59-75.
- [2] T. Castillo, A. García, C. Padilla-Córdova, A. D. Barrera, C. Peña, *Electronic Journal of Biotechnology* 48 (2020) 36-45.

### Acknowledgement

This work was supported by the Grant Agency of the Czech Republic (GAČR project GA23-06757S). Martin Súkeník, Brno Ph.D. Talent scholarship holder - funded by the Statutory City of Brno.

## PW22: The Interaction of Hazardous Metals - Microplastics

### Sinčáková Lenka<sup>1</sup>, Ottová Michaela<sup>1</sup>, Doležalová Weissmannová Helena<sup>1</sup>

<sup>1</sup> BUT, Faculty of Chemistry, ICTEP, Purkyňova 118, Brno, 612 00, Email: dolezalova@fch.vutbr.cz

### Keywords: hazardous metals, microplastics, polyethylene terephthalate, fresh water, sea water

Microplastics are a long-term, significant threat to the environment as well as organisms, and are nowadays ubiquitous in the environment. Among all environmental realms, the hydrosphere stands out as a primary reservoir for the majority of microplastics.

Due to several specific properties (small particle size combined with large surface area, hydrophobicity), microplastics tend to adsorb several hydrophobic substances on their surface from the environment [1, 2]. Among substances commonly found adsorbed on the microplastics surface is 78 % of chemicals listed as "priority pollutants" by Environmental Protection Agency (EPA) (bioaccumulative, persistent and/or toxic). Unlike organic compounds, the presence of metals adsorbed on microplastics has been studied for a significantly shorter time [3].

Experiments were performed with 5 common heavy metals (Pb, Hg, Zn, Cu and Cd) and PET, a widespread polymer, with the use of atomic absorption spectrometry (F AAS, GF AAS). Experiments were carried out in two laboratory prepared environments (fresh water and sea water), that aimed to stimulate real-world conditions. The polymer was used in two fractions - small fraction (<0.63  $\mu$ m) and big fraction (0.63  $\mu$ m-1 mm) to illustrate impact of MP particles size on the adsorption process.



Figure 1: Interaction of of different types of microplastics with HMs [4]

### References

- [1] M. G. Kutralam, F. Pérez Guevara, I. E. Martínez, V. Shruti, Journal of Hazardous Materials 415 (2021) 125755.
- [2] Q. An, T. Zhou, C. Wen, C. Yan, Journal of Hazardous Materials 460 (2023) 132369.
- [3] N. Khalid, M. Aqeel, A. Noman, S. M. Khan, N. Akhter, Environmental Pollution 290 (2021) 118104.
- [4] L. Fu, J. Li, G. Wang, Y. Luan, W. Dai, Ecotoxicology and Environmental Safety 217 (2021) 112207.

### Acknowledgement

The work was supported by the project FCH-S-24-8591 of Ministry of Education, Youth and Sports of the Czech Republic.

The differences between small and big fraction varied among the metals, with no clear observable trend. This suggest that other factors than the size of the active surface of MPs, played more prominent role. With regards to the water conditions, increased ionic strength in sea water clearly hindered adsorption process, which can be attributed to phenomena such as competition for adsorption sites, electrostatic repulsion, MPs aggregation and formation of complexes. All data have been fitted with Langmuir, Freundlich and Temkin adsorption isotherms.

The determined preferred adsorption models vary - Zn follows the Freundlich adsorption model the most, Hg and Cd follow the Langmuir adsorption model, while Pb and Cu yield best results with Temkin adsorption model. Considering the maximal adsorbed amounts (and therefore, the adsorption capacity of PET for the given metal), metals can be ordered as follows: Hg < Cd < Zn < Pb < Cu. While the sorption of hydrophobic organic pollutants in aquatic environments is well documented, the sorption of heavy metals remains poorly understood. The differences in adsorption processes for varying ionic strength conditions demonstrate the importance of further research on the adsorption of heavy metals on microplastics regarding the environmental conditions they occur in real life. This means considering the factors as environment and MPs condition, studying the HMs adsorption on MPs regarding other entities present in the aquatic environment, such as other contaminants (i.e., organic pollutants), microorganisms and organic matter, among others, and using real, collected weathered microplastics, as those tend to have higher adsorption capacities. In some of the experiments, the adsorption curves have not fully reached the plateau stage yet, indicating higher concentrations might be needed in future experiments.

# PW23: The Study of the Content of Risk Elements in Power Plant Ash

### Komendová Renata<sup>1</sup>, Vlčková Renáta<sup>1</sup>

<sup>1</sup> Institute of Chemistry and Technology of Environmental Protection, Faculty of Chemistry, Brno University of technology, Purkyňova 118, 61200 Brno, Czech Republic, Email: komendova@fch.vut.cz

### Keywords: brown coal, biomass, bad ash, fly ash, risk elements, ETAAS

Burning coal is an important source of energy, but it carries with it several risks, namely CO2, NOx and SOx emissions. Renewable sources have started to be used to reduce these emissions. One of the renewable sources is biomass, which is burned together with brown coal. The co-combustion of brown coal and biomass has shown positive results in reducing emissions (CO<sub>2</sub> and SO<sub>x</sub>). Biomass is considered a carbon-neutral fuel because it absorbs a large amount of CO<sub>2</sub> from the atmosphere as a result of photosynthesis. The basic components of coal and biomass are the elements C, H, O, N and S. Coal also contains risk elements such as Hg, Pb, Cr and Cd. By burning coal, these hazardous elements are then released into the flue gas and subsequently released into the air, from which they can enter the soil, water sources and the food chain. For this reason, technologies have been developed for flue gas cleaning, such as cyclone separators, electrostatic separators or fabric or ceramic filters. The generated secondary energy products, which include fly ash and bed ash, are deposited in an ash sludge disposal facility or are treated as a product.

This study deals with the determination of the content of the risk elements Hg, Cr, Pb and Cd in the samples provided by Thermal Power Plant X. During the annual monitoring, samples of brown coal, biomass, fly ash, bed ash, water from the tailings pond and river water used for cooling were sampled every month. Atomic absorption spectrometry (AMA 254 and ETAAS) was used for the determination. Concentrations of risk elements in brown coal and biomass samples decrease in the order Cr > Pb > Hg > Cd, and in fly ash and bed ash samples decrease in the order Cr > Pb > Cd > Hg. Overall, it was evaluated that the contents of risk elements after the co-combustion of brown coal and biomass passed mainly into the fly ash and less into the bed ash. It was found that by burning a higher amount of biomass, the content of Hg, Cr and Pb in fly ash and bed ash decreased. The water samples were classified as unpolluted water according to the specified parameters. In general, thermal power plants are still currently a source of pollution, not only in the locality of their operation, but also in terms of long-distance transport of pollutants. Although Thermal Power Plant X complies with the emission limits, its operation is an anthropogenic source of air pollution in the long term.



Figure 1: A) brown coal, B) biomass, C) bed ash, D) fly ash

# PW24: Thin Porous Carbon Layers on Ceramics for Environmental Applications

### Perveen Sajida<sup>1</sup>, Slovák Václav<sup>1</sup>

<sup>1</sup> University of Ostrava, Faculty of Science, Department of Chemistry, 30. dubna 22, 702 00 Ostrava, Email: sajida.ali028@gmail.com

### Keywords: porous carbon, thin layer, ceramics, adsorption

Biomass based activated carbons present a common adsorbent for decontamination of environment. Despite its undeniable advantages, its use is also associated with problems. Powdered activated carbon is difficult to separate, and the pelletized form has much poorer adsorption properties. The solution may be to prepare layers of porous carbon on a suitable support.

In this research, several methods of synthesis of thin porous carbon layers on ceramic foam as a support were tested.

The dip-coating of pieces of ceramic foam made of  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> with suitable carbon precursors was adopted as a basic approach.

As a main precursor, commercial wood tar in a mixture with formaldehyde (sample TS) and HCl (THS), oxalic acid (TOS) or both (THOS) was used [1]. For comparison, sucrose (Sc) [2] and phloroglucinol (PGS) [3] solutions were also tested. All prepared materials were carbonized at 500 °C for one hour in a flow of nitrogen.

Combustion analysis showed that the prepared materials varied in carbon content (w/w) - TS (2.45%), THS (1.6%), TOS (1.6%), THOS (1.49%), Sc (9.85%), PGS (4.23%). Although Sc showed the highest amount of carbon, the surface layer was brittle and peeled off very easily. The other samples showed a good mechanical stability.

Porosity of prepared materials was characterized by iodine adsorption. Comparing the results with substrate itself showed increased porosity of samples equipped with carbon layer (PGS>Sc>TS>THS>THOS>TOS).

Application testing was realized as adsorption of methylene blue (MB) from aqueous solution (50 mL, 15  $\mu$ mol/L, 1 piece of adsorbent, stirring, 40 minutes).

### References

- [1] W.M. Qiao, et.al., *Energy & Fuels* 19 (2005) 2576.
- [2] L. Wei, N. Nitta, G. Yushin, ACS Nano 7 (2013) 6498.
- [3] S. Kataoka, et.al., Colloids Surf. A 347 (2009) 142.

### Acknowledgement

This work was supported by the students' project SGS09/PŘF/2024 (University of Ostrava).

Determined absolute adsorbed amount of MB per one piece of tested material was recalculated to a gram of carbon present in the surface layer (Figure 1).



Figure 1: Adsorbed amount of methylene blue on prepared samples (related to g of carbon present in surface layer)

Sucrose based sample was found to be the best adsorbent under given conditions. Considering its mechanical instability, for practical applications the wood tar-based samples seem to be better. Surprisingly, preparation without any catalyst (sample TS) provides the most efficient adsorbent in this series.

This study concludes the applicability of biomass tar for very simple making thin and porous carbon layers on the ceramic support. Optimizing the synthetic procedure promises obtaining cheap, efficient and easy to handle adsorbent for water remediation.

# PW25: The Interaction of Microplastics and Microbioplastics with Soil and a Comparison of Their Potential to Spread Pathogens

Trojan Marek<sup>1,</sup> Koutný Marek<sup>2</sup>, Brtnický Martin<sup>3,</sup> Holátko Jiří<sup>3</sup>, Zlámalová Gargošová Helena<sup>1</sup>, Fojt Jakub<sup>4</sup>, Procházková Petra<sup>1</sup>, Kalčíková Gabriela<sup>5</sup>, Kučerík Jiří<sup>3</sup>

- 1 Institute of Chemistry and Technology of Environmental Protection, Faculty of Chemistry, Brno University of Technology, 612 00 Brno, Czech Republic, Email: marek.trojan1@vutbr.cz
- Department of Environmental Protection Engineering, Faculty of Technology, Tomas Bata University in Zlín, 760 01 Zlín, Czech Republic
- 3 Department of Agrochemistry, Soil Science, Microbiology and Plant Nutrition, Mendel University in Brno, 613 00 Brno, Czech Republic
- Textile Testing Institute, Cejl 480/12, 602 00 Brno, Czech Republic
- Faculty of Chemistry and Chemical Technology, University of Ljubljana, 1000 Ljubljana, Slovenia

### Keywords: microplastics, biodegradation, bioplastics, vectors, pathogen, soil

Microplastics contribute to various environmental issues and serve as carriers for a wide range of toxic compounds such as pesticides, pharmaceuticals, and metal ions. Consequently, there is a gradual shift towards replacing them with biodegradable plastics (bioplastics). However, biodegradable plastics require specific conditions for complete biodegradation, and their biodeterioration often leads to the rapid production of smaller fragments, known as microbioplastics.

In this poster, we summarize selected issues related to the impact of plastic particles on soil properties and the soil microbiome. Findings from numerous studies indicate that both microplastics and microbioplastics induce adverse changes in soil microbiology, potentially increasing the abundance of soil-borne pathogens. Based on these observations, we argue that plastic particles could serve as carriers for colonies of soil-borne pathogens.

Furthermore, the use of bioplastics may exacerbate this issue due to their easier and faster formation,

Acknowledgement

This poster is based upon work from COST Action CA20101 Plastics monitoRIng detectiOn RemediaTion recovery-PRIORITY, supported by COST (European Cooperation in Science and Technology, www.cost.eu, accessed on 22 May 2024).

increased support for biofilms, and more pronounced adverse effects on soil biota. However, further research is necessary to either substantiate or refute this perspective.



*Figure 1: Illustration of the view described in the poster.* 

## PW26: Macro and Micro Views of Pressure Membranes Used for Wastewater Treatment

### Vespalec Jan<sup>1</sup>, Repková Martina<sup>1</sup>, Figalla Silverstr<sup>1</sup>

<sup>1</sup> Brno University of Technology, Faculty of Chemistry, Department of Chemistry and Technology of Environmental Protection, Purkyňova 464/118, 612 00 Brno, Czech Republic, Email: Jan.Vespalec@vut.cz

Keywords: reverse osmosis membranes, nanofiltration membranes, ultrafiltration membranes, membrane fouling

The membranes gradually become fouled when water is treated using pressure separation processes. Fouling occurs in all types of membranes (Microfiltration - MF, Ultrafiltration - UF, Nanofiltration - NF and Reverse Osmosis - RO). Fouling is a normal part of membrane operation. Backwash, forward flush, or, in a more extreme situation, Clean in Place (CIP) is regularly performed before fouling. However, the CIP process is less gentle on the membrane due to the use of aggressive chemicals [1,2]. To reveal what the membranes are contaminated with, we used scanning electron microscopy (SEM) as one of the methods.

Figure 1 is an SEM image of the reverse osmotic membrane from the permeate side (i.e., the permeate drain side). Figure 2 is an SEM image of the cleaned reverse osmotic membrane from the concentrate side (i.e., the influent and effluent side of the concentrate).



Figure 1: Surface of the reverse osmosis membrane from the permeate side



Figure 2: Surface of the cleaned reverse osmosis membrane from the concentrate side

Using electron microscope images, we can detect mechanical wear on the membrane and determine how much contamination remains after the CIP method. Using SEM mapping, we can obtain images showing the middle layer of the RO membrane, which is composed of microporous polysulfone. This allows us to distinguish worn or fouling clogged areas on the membrane. The most common reason for clogging is organic matter covering the entire membrane on the concentrate side. In addition, carbonates and residues of coagulant and antiscalant are most likely.

The current goal is to map the membranes and determine what pollution is fouling them. These were membranes where even the CIP method no longer helped. Continued research on the membranes will test appropriate membrane-cleaning procedures.

.....

### References

- [1] J. C. Crittenden, R. R. Trussell, D. W. Hand, K. J. Howe, G. Tchobanoglous, *MWH's Water Treatment*, Hoboken, NJ, USA: John Wiley & Sons, 2012.
- [2] D. Mackenzie, in: Water and Wastewater Engineering: Design Principles and Practice, 2019, p. 455–475.

### Acknowledgement

The work was supported by the projects CZ.01.01/06/23\_014/0001373 and FCH-S-24-8591 Ministry of Education, Youth and Sports of the Czech Republic.

# PW27: Innovative Integration of High-Resolution Mass Spectrometry and In-Silico Libraries for Pharmacetical Metabolite Identification in Lettuce (*Lactuca sativa*)

**Fučík Jan<sup>1</sup>**, Fučík Stanislav<sup>2</sup>, Rexroth Sascha<sup>3</sup>, Hamplová Marie<sup>1</sup>, Navrkalová Jitka<sup>1</sup>, Zlámalová Gargošová Helena<sup>1</sup>, Mravcová Ludmila<sup>1</sup>

- <sup>1</sup> Institute of Chemistry and Technology of Environmental Protection, Faculty of Chemistry, Brno University of Technology, Purkyňova 118, 612 00 Brno, Czech Republic, Email: xcfucikj@vutbr.cz
- <sup>2</sup> Faculty of Electrical Engineering and Communication, Brno University of Technology, Technická 3058/10, 616 00 Brno, Czech Republic
- <sup>3</sup> Shimadzu Europa GmbH, Albert-Hahn-Straße 6, 472 69 Duisburg, Germany

Keywords: pharmaceutical metabolites; structure prediction; in silico spectral library; liquid chromatography; high-resolution mass spectrometry

Lettuce, as one of many types of edible vegetables, is often grown hydroponically to maximize yield, reduce soilrelated issues, and save water. Given that lettuce is composed of 95% water, it is particularly well-suited for hydroponic cultivation. This method frequently utilizes wastewater, which is cost-effective and sustainable. However. such water can be contaminated with pharmaceuticals, in some cases as up to 90% of ingested medication is excreted in its original form. Additionally, wastewater may contain metabolites and degradation products of these pharmaceuticals. All of these substances can be absorbed by the crops, particularly through their roots. This can lead to the translocation of these compounds into the leafy edible parts of the lettuce. Furthermore, the presence of pharmaceuticals in the water can lead to the formation of further metabolites.

This contamination not only fosters the emergence of antimicrobial resistance but also presents health risk

due to prolonged exposure to these residues. However, current monitoring practices often focus solely on quantifying parent drugs, leading to an underestimation of health risks associated with the consumption of grown vegetables.

Therefore, the novelty/benefit of this study lies in the development of a novel high-throughput workflow for identifying pharmaceutical metabolites (Met-ID) using LC-HRMS. Unlike commercially available software, our approach utilizes our own python script and opensource software with accessible algorithms, allowing for scientific scrutiny and validation of the process. Specifically, software tools were utilized for: 1) Metabolite structure prediction, 2) In Silico spectral library prediction, 3) Data processing, and 4) Statistical data evaluation. Additionally, LC-qTOF measurements were conducted in both ESI+ and ESI- modes, employing both Data-Dependent Acquisition (DDA) and Data-Independent Acquisition (DIA) modes to assess their efficacy in Met-ID.



Figure 1: High-Throughput Workflow for Pharmaceutical Metabolite Identification in Lettuce Samples

### Acknowledgement

This research was financially supported by the Ministry of Education, Youth, and Sports of the Czech Republic (Project No. FCH-S-24-8591) and samples were analysed within the Lab4you Shimadzu student program in 2022. Furthermore, we acknowledge that the graphical abstract was created in BioRender.

# PW28: Adsorption Behaviour of Hyaluronan Derivatives with Reduced Carboxyl Groups at Charged Hydrophobic Surface

### Fojtíková Jana<sup>1</sup>, Ondreáš František<sup>2</sup>, Švecová Eliška<sup>3</sup>

<sup>1</sup> Faculty of Chemistry, Brno University of Technology, Institute of Physical and Applied Chemistry, Purkyňova 464/118, 612 00 Brno, Czech Republic, Email: Jana.Fojtikova1@vut.cz

Keywords: hyaluronan derivatives, AC voltammetry, adsorption/desorption, electrostatic interactions, hydrophobic interactions

Hyaluronan is negatively charged polysaccharide and is one of the main components of extracellular matrix of all vertebrates, thus it is without doubt, that interactions of hyaluronan with charged biological surfaces, such as cell membranes, have an essential role in *in vivo* processes. Despite that, relatively little information exists on the adsorption of hyaluronan.

In recent study was shown, that phase-sensitive alternating current voltammetry in phase-out mode can be used to study adsorption and desorption behavior of polysaccharides that do not contain redox centre or free amine group, such as hyaluronic acid [1]. This method allows separation of faradaic and capacitive electric current components as a function of electrode potential. Changes in capacitive current indicate adsorption/desorption processes occurring in the solution. Hanging mercury drop electrode is most commonly used because of its hydrophobic surface, which enables measurements of not only electrostatic interactions but also hydrophobic.



Figure 1: Voltammogram of native hyaluronan in acetate buffer

### References

- [1] E. Švecová, V. Ostatná, L. Fojt, M. Hermannová, V. Velebný, F. Ondreaš, Carbohydrate Polymers 277 (2022) 118831.
- [2] J. Fojtíková. *Effect of reduction of carboxyl groups on the physicochemical properties of hyaluronan*. FCH VUT, Czech Republic, 2024.

### Acknowledgement

This study was performed in collaboration with Contipro a.s..

In the present study we use this method to observe adsorption and desorption processes of native hyaluronan and reduced hyaluronan derivatives at charged hydrophobic interface of mercury electrode in different buffered solutions. Electrostatic and hydrophobic interactions were distinguished for native hyaluronan as well as for its reduced derivatives.

In accordance with our assumptions, hydrophobic interactions are more prominent in derivatives, while electrostatic in native hyaluronan. Moreover, in the case of derivatives the shape of voltammograms corresponds to the degree of reduction, with the most distinct differences in the area of hydrophobic interactions. Subsequently, adsorption isotherms of native hyaluronan and its reduced derivative were plotted, and critical concentration of saturation was obtained for both samples.

Results showed that reduction of carboxyl groups in hyaluronan enables its chains to form stronger hydrophobic interactions with each other or with other polymers or surfaces at a price of slightly weaker electrostatic interactions in comparation to native hyaluronan. This also means weaker repulsive electrostatic interactions between chains with the same charge which leads to higher viscosity above the concentration of entanglement and better mucoadhesion compared to native hyaluronan [2].

Based on these findings we can conclude that the reduction of carboxyl groups led to such changes in derivatives properties that noticeably increase its application potential in suitable indications, such as viscosuplementation or ophthalmology [2].

# PW29: Exploring Intermolecular Interactions in Aqueous γ-Valerolactone Mixtures with a Combination of Molecular Dynamics Simulations and Experimental Techniques

### Jeřábek Vojtěch<sup>1</sup>, Heyda Jan<sup>1</sup>, Řehák Karel<sup>1</sup>

<sup>1</sup> University of Chemistry and Technology, Department of Physical Chemistry, Technická 5, CZ-16628 Prague 6, Czech Republic, Email: jerabekv@vscht.cz

Keywords: γ-valerolactone, intermolecular interactions, molecular dynamics, thermodynamics of mixtures

One of the directions of the current chemistry is the creation of environmentally friendly processes and the production of chemicals from renewable resources. For these purposes, so-called green solvents, substances with low or zero toxicity that can be produced from renewable sources, appear to be suitable candidates. One of the most promising green solvents is y-valerolactone (GVL, see Fig. 1), which can be obtained by processing lignocellulose, the most abundant renewable biopolymer on Earth [1]. Aqueous mixtures of green solvents are also of interest due to a phenomenon called hydrotropy, i.e., increase in the solubility of hydrophobic substances by adding small amounts of water to a pure organic solvent [2-3]. Hydrophobic substances (e.g., pharmaceuticals, natural substances, or biopolymers) represent an industrially important class of compounds, which solvation and dissolution is, however, a complex process. Complete characterization of macroscopic properties of hydrotropes mixtures and understanding of their microscopic structure driving interactions and forces is essential to understand the mechanism of solvation and dissolution action.

In this work, a combination of theoretical and experimental approaches was applied to study aqueous GVL mixtures over the entire composition range and at temperatures of 278-328 K. The volumetric, transport, thermodynamic and structural properties of these solutions were studied, in particular the excess volume, viscosity deviation, diffusion and activity coefficients. Utilizing novel experimental data, a thermodynamically consistent microscopic model was obtained which in turn provides insight into solution structure (spatial and radial distribution functions) and points to the key interactions occurring in these systems at the atomic level.

The microscopic insight relies on molecular dynamics (MD) simulations using GROMACS software. Evaluation of MD trajectories provided the structural and macroscopic

### References

- [1] C. López-Aguado, D. M. del Monte, M. Paniagua, G. Morales, J. A. Melero, Ind. Eng. Chem. Res. 61 (2022) 5547.
- [2] D. O. Abranches, J. Benfica, S. Shimizu, J. A. P. Coutinho, Ind. Eng. Chem. Res. 59 (2020) 18247.

[3] M. de Bruyn, V. L. Budarin, A. Misefari, S. Shimizu, H. Fish, M. Cockett, A. J. Hunt, H. Hofstetter, B. M. Weckhuysen, J. H. Clark, D. J. Macquarrie, *ACS Sustain. Chem. Eng.* 7 (2019) 7878.

### Acknowledgement

This work was supported from the LUABA24070 project and the grant of Specific university research – grant No. A1\_FCHI\_2024\_001.

properties of studied solutions. The experimental part consisted in directly measuring the density, viscosity and thermodynamic activity of aqueous mixtures, evaluating the corresponding derived quantities and describing them using appropriate models (Redlich-Kister expansion, thermodynamic models based on excess Gibbs energy).

Based on the thermodynamic results obtained, it can be concluded that several specific interactions occur in GVL/water mixtures, leading to significant deviations from the ideal behavior. Moreover, the results of MD simulations indicate presence of a strong anisotropies in GVL hydration and solvation and potential existence of transient nanostructures in solution. The knowledge of GVL/water mixtures behavior can lead to better understanding of the hydrophobic compounds' dissolution mechanisms, design and optimization of sustainable processes at desired conditions.



Figure 1: Strong anisotropy of spatial distribution of the GVL carbonyl oxygen (gold) and of the water molecule (oxygen in red, hydrogen in white) around the GVL molecule at 10mol% mixture

# PW30: Application of Macro- and Microrheology for Cerebrospinal Fluid Under Different Temperature Conditions

**Bradt Elke**<sup>1</sup>, Bauer Thessa-Carina<sup>1</sup>, Hild Sabine<sup>1</sup>, Gruber Andreas<sup>2</sup>, Rossmann Tobias<sup>2</sup>, Ruiz-Navarro Francisco<sup>2</sup>, Oberndorfer Johannes<sup>2</sup>, Stefanits Harald<sup>2</sup>, Kracalik Milan<sup>1</sup>

- <sup>1</sup> Johannes Kepler University Linz, Institute of Polymer Science, Altenberger Str. 69, 4040 Linz, Austria, Email: Elke.Bradt@jku.at
- <sup>2</sup> Kepler University Hospital, Department of Neurosurgery and Johannes Kepler University Linz, Faculty of Medicine, Clinical Research Institute for Neurosciences, Wagner-Jauregg-Weg 15, 4020 Linz, Austria

### Keywords: microrheology, cerebrospinal fluid, macrorheology

Rheology of viscoelastic materials is considered to determine the amount of elastic and viscous response for better understanding the behavior at processing as well as application conditions. Nowadays this method is also used in the biological field, since biofluids consist of an aqueous solution with certain long chain macromolecules, as proteins among others. The flow behavior of fluent materials can provide information about the amount of viscous or elastic molecular movement. According to different measuring types rheology can be divided into macro- and microrheology.

Macrorheology is an active operating method, referring to the measuring mode either the shear stress is applied and the shear rate is determined or vice versa. For small shear rates marcrorheology provides valuable information.

Comparing to marcrorheology, passive microrheology is a non-destructive method, using tracer particles driven by thermal energy (Brownian motion) which applies only minimal deformation to the estimated medium. This method is interesting for the biological field, due to the fact that the measuring process only needs some  $\mu$ l sample volume. Microrheology offers data in higher shear rate range than macrorheology, therefore the data of both methods are complementary.

In our study, cerebrospinal fluid (CSF) from patients after subarachnoid hemorrhage (SAH) was analyzed using macro- and microrheology at physiological relevant temperatures. Different conditions in the human body were simulated by measuring the samples at these specific temperatures (5°C, 35°C, 37°C, 40°C), as the storage temperature in refrigerator – undercooled – physiologic – and elevated body temperature.

The results were compared between these two methods and opposed with preliminary correlations between macrorheological and laboratory parameters of cerebrospinal fluid. These studies show, that there are dependencies on certain disease patterns of patients, as well on the time elapsed since subarachnoid hemorrhage.

### Acknowledgement

We would like to express our gratitude for the financial support provided by Impetus, Faculty of Medicine at Johannes Kepler University Linz, project number: MP0116101001 and LIT Institute of Technology at Johannes Kepler University Linz, project number: LI113490001.

# PW31: Rheological Characterization of Hydrogel Materials Using Oscillatory Rheometry and Microrheological Technique Fluorescence Correlation Spectroscopy

### Kadlec Martin<sup>1</sup>, Obrusníková Klára<sup>2</sup>, Smilek Jiří<sup>3</sup>

<sup>1</sup> Brno University of Technology, Faculty of Chemistry, Institute of physical and applied chemistry, Purkyňova 464/118, CZ-612 00 Brno, Czech Republic, Email: Martin.Kadlec@vut.cz

### Keywords: rheology, fluorescence correlation spectroscopy, hydrogels, agarose, gellan

Hydrogels are unique disperse systems consisting of three dimensional network of cross-linked polymers and aqueous environment [1]. These materials are nowadays often utilized in food industry as gelling agents and stabilizers, however, they are also increasingly used in the areas of tissue engineering, as wound dressing, drug delivery systems or as scaffolds, since these materials are often biocompatible and biodegradable [2, 3]. Moreover, due to their similar properties to living tissues (high water content, favorable mechanical properties), hydrogels can be utilized also as materials imitating extracellular matrix (ECM) [4, 5].

Since hydrogels are materials, which usually report viscoelastic behavior, they are commonly studied via oscillatory rheological measurements, where the sample is studied in its bulk form. However, rheological properties can be also studied by the methods, so called microrheological methods. In this case we are gathering valuable rheological information about the studied samples on their microscale by tracking a probe incorporated into the hydrogel. These information are of a great interest for example for gel-like materials utilizing as potential drug carriers or ECM models, since the local rheological behavior is closely related to the transport through the gel

In this presented study, rheological properties of gellan and agarose hydrogels were studied by the marcoas well as microrheological approach. In case of the microrheological technique, fluorescence correlation spectroscopy (FCS) was utilized.

From the obtained results for gellan hydrogel (Figure 1), it can be seen, that the microrheological approach substantially extended the range of the frequency in which the viscoelastic moduli can be studied. From the macrorheological point of view, the material behaves like a viscoelastic solid in the whole frequency range measured, since the storage modulus is higher than

the loss modulus. On the other hand, from the gathered FCS data in the lower frequencies, gellan gel reports viscoelastic liquid behavior roughly up to 1 Hz. After exceeding this point, crossover of moduli can be observed, followed with the domination of storage modulus over the loss modulus. FCS also underestimates the values of both the storage and loss moduli by two orders of magnitude when comparing to macrorheological approach. That could cohere to the way the sample is viewed. The microrheological probe of the size 50 nm "sees" the microstructural elements of the sample, which could be much more compliant than the whole structure, which is studied via the parallel plates of the rheometer.



Figure 1: Comparison of viscoelastic moduli of 1% gellan gel obtained by FCS and macrorheology

In conclusion, it should be noted, that both the macrorheological and microrheological approach provide valuable information about the mechanical properties when studying hydrogel materials, since each of the approaches study the sample in a different way. Finally, comprehensive rheological characteristics can be obtained when utilizing both of them.

### References

- [1] F. Ullah, M. B. H. Othman, F. Javed, Z. Ahmad, H. Akil, Materials Science and Engineering: C.57 (2015), 414-433.
- [2] A. Awadhiya, S. Tyeb, K. Rathore, V. Verma, Engineering in Life Sciences 17 (2017) 204-214.
- [3] B. L. Roach, A. B. Nover, G. A. Ateshian, C. T. Hung, *Biomaterials from Nature for Advanced Devices and Therapies*. Hoboken, New Jersey, 2016, 258-273.
- [4] X. Yan, Q. Chen, J. An, et al. Journal of Materials Chemistry B 7 (2019) 95-102.
- [5] A. Canibano-Hernández, L. Saenz del Burgo, A. Esponanoguera, G. ORIVE, R. M. Hernández, J. Ciriza, J. L. Pedraz, Molecular Pharmaceutics 14 (2017) 2390-2399.

# PW32: Alternative Crosslinking Methods for Sodium Alginate Resulting in Hydrogels with Suitable Application Properties

### Kouřilová Ludmila<sup>1</sup>, Smilek Jiří<sup>2</sup>, Kadlec Martin<sup>3</sup>

<sup>1</sup> Faculty of Chemistry, Brno University of Technology, Institute of Physical and Applied Chemistry, Purkyňova 464/118, 612 00 Brno, Czech Republic, Email: Ludmila.Kourilova@vut.cz

### Keywords: sodium alginate; polysaccharides; hydrogels; rheology; viscoelastic properties

Sodium alginate represents a pioneer gel-forming component in the field of materials engineering, known for its unique capabilities such as high biocompatibility, low toxicity, and especially its ability to form strong, flexible gel structures with excellent stability. This polymer was the focus of the present study, which deals with the preparation of alginate gels with the potential to influence their final application properties (transparency, syneresis, viscoelastic properties, etc.). Two strategies were selected leading to the gelation of sodium alginate, namely ionic cross-linking by the external gelation method (diffusion of calcium ions into the alginate sol) and ionic cross-linking by the internal gelation method (delayed gelation using limited soluble calcium salt and D-glucono- $\delta$ -lactone).



Figure 1: Scheme of ionic cross-linking of alginate by the internal gelation method.

Subsequently, optimization of the preparation of alginate gels was performed, their mechanical properties were characterized using selected rheometric tests (amplitude sweeps with shear deformation and time sweeps), and finally, the influence of several factors (polymer concentration, amount of cross-linking agent, gelation time, addition of sucrose, etc.) on the final properties of the prepared gels was investigated.

It has been demonstrated that as the polymer concentration decreases, the mechanical strength of the gels also decreases, while, for example, the transparency of gels with lower polymer concentrations increases. The amount of cross-linking agent used plays an important role; with its addition, the degree of cross-linking increases, and consequently, the mechanical strength of the alginate gel also increases. The final properties of the hydrogels can also be influenced by the gelation rate, which affects, for example, their homogeneity (gels formed at a higher gelation rate tend to be less homogeneous). In the presented work, it was possible to slow down the gelation rate by adding phosphate ions, which led to higher homogeneity of the prepared gels but did not significantly affect their mechanical properties.

A major issue in the preparation of hydrogel materials is also a phenomenon known as syneresis, which is generally undesirable. The present work demonstrated that, in some cases, this phenomenon can be slowed down by adding sucrose to the alginate sol before gelation. Another significant contribution of this work is the finding that, in ionic cross-linking of alginate by the external gelation method, not only the type of cation affects the final properties of the gels, which is a well-known fact, but in some cases, the type of anion used also influences the final properties of the gels.

An interesting part of the work is also the optimization of the analysis of the mechanical properties of alginate gels through compression tests. During these tests, the sample is compressed in the rheometer between two planar sensors, and the normal force exerted by the sample on the upper plate of the rheometer is recorded. This is one of the most easily visualizable rheometric tests.



Figure 2: Squeeze tests performed on alginate beads at different sample compression speeds.

### References

[1] L. KOUŘILOVÁ, Alternative Methods of Cross-linking Sodium Alginate Leading to Hydrogels with Suitable Application Properties. Brno University of Technology, Faculty of Chemistry, Brno, Czechia, 2024.

### Acknowledgement

This work was supported by the Grant Agency of the Czech Republic (GAČR project GA23-06757S).

## PW33: Hybrid Gellan Hydrogels – Preparation and Characterization

### Krouská Jitka<sup>1</sup>, Borovský Martin<sup>1</sup>, Kalina Michal<sup>1</sup>

<sup>1</sup> Faculty of Chemistry, Brno University of Technology, Purkynova 118, 612 00 Brno, Czech Republic, Email: krouska@fch.vut.cz

### Keywords: hybrid hydrogel, gellan, reometry, multivalent ions

One way how to prepare hybrid hydrogels is the gelation of a natural polymer and a synthetic crosslinking agent. These materials with high water content could have wide field of applications: in drug delivery, as scaffolds, in tissue engineering or regenerative medicine. The most important parameter is the mechanical resistance of these materials to external influences depending on the specific application therefore the optimal conditions in preparation of these materials are crucial.

The aim of this work was to prepare hybrid gellan hydrogels based on the combination of physical crosslinking and ionic interaction of the functional groups of gellan (Figure 1) with multivalent ions of selected metals.



Figure 1: Gellan structure

The hydrogel samples (one example in Figure 2) were characterized by rheometry to obtain information about the mechanical properties. The additional swelling behavior was tested in distilled water and the rate of drying was determined using the drying scales.



Figure 2: Illustration of gellan hydrogels crosslinked with  $Fe^{3+}$  ions.

It was found that the hydrogels with the addition of multivalent ions exhibit a higher degree of crosslinking of the network which positively affects the resulting mechanical properties of the hydrogels. Those properties could be modified using different ions and their concentration to obtain suitable hydrogel material for subsequent application.

# PW34: Structural Characterization of Monomer Composition of Sodium Alginate by Vibrational Spectroscopy

### Přibyl Jiří<sup>1</sup>, Sedláček Petr<sup>1</sup>, Kianička Michal<sup>1</sup>

<sup>1</sup> Brno University of Technology, Faculty of Chemistry, Institute of Physical and Applied Chemistry, Purkyňova 464/118, 612 00 Brno, Czech Republic, Email: Jiri.Pribyl1@vut.cz

### Keywords: Sodium alginate, ATR-FTIR, Raman microspectroscopy, Sustainable agriculture

In recent years, there has been growing interest in developing novel chemical and biological soil amendments within the framework of sustainable agriculture. One of the revolutionary approaches in the production of soil bioinoculants is represented by the recently proposed selfentrapment of Plant Growth Promoting Rhizobacteria (PGPR) by gelation of their own extracellular polysaccharides. A common method for the gelation of sodium alginate involves the use of multivalent cations, such as calcium ions ( $Ca^{2+}$ ), which facilitate cross-linking and network formation within the alginate structure. However, the efficiency of alginate gelation and the stability of resulting gels depends on three critical structural parameters of the polymer: molecular weight, (de)acetylation, and monomer composition. These factors influence the physical properties of the resulting hydrogel, including its strength, porosity, and biodegradability, which are crucial for its effectiveness as a carrier for PGPR. Understanding and optimizing these parameters can enhance the functionality and reliability of alginate-based bioinoculants. The characterization of the monomer composition is the focus of this work.

For the study of the monomer composition of sodium alginate, which is made up of L-guluronic acid blocks (poly-G) and D-mannuronic acid blocks (poly-M), the methods of ATR-FTIR, RAMAN microspectroscopy, and FT-RAMAN spectroscopy were utilized. Initially, a series of calibration

samples were prepared from mixtures of commercial standards of poly-G and poly-M. These samples provided a controlled basis for analysis, allowing for precise measurement of spectral data. The obtained results were analyzed by principal component analysis (PCA), the method that determines the directions of the highest variability within the spectral data. PCA facilitated the identification of two significant peaks corresponding to the monomeric composition's influence on the analyzed spectra. These were observed peaks at wavelength 820 and 950 cm<sup>-1</sup>. The ratio of these peaks was found to correlate with the known content of poly-G in each calibration sample. Consequently, calibration curves were constructed for all tested spectroscopic techniques, enabling the quantification of poly-G concentration in commercial sodium alginate samples. In conclusion, while our study presents a promising method for determining the poly-G concentration in sodium alginate using techniques of vibrational spectroscopy, further research is needed to validate and refine this approach. Exploring additional methodologies will be crucial in confirming our findings and improving the accuracy and reliability of this analytical technique, ultimately contributing to more precise characterizations of sodium alginate in various applications, including research and development of alginate-based bioinoculants.

### Acknowledgement

This work was supported by the Grant Agency of the Czech Republic (GAČR project GA23-06757S).
# PW35: Targeted Functionalization of Atomic Force Microscopy Tips for the Study of Polysaccharide Hydrogel Systems

#### Smilek Jiri<sup>1</sup>, Liskova Katerina<sup>1</sup>, Kadlec Martin<sup>1</sup>

<sup>1</sup> Brno University of Technology, Faculty of Chemistry, Purkynova 464/118, 612 00 Brno, Czech Republic, Email: smilek@fch.vut.cz

#### Keywords: atomic force microscopy, hydrogel, force spectroscopy, polysaccharides, Young's modulus

Atomic force microscopy (AFM) is a unique, highresolution imaging technique which allows to investigate the surface topography of various (including semi-solid) materials at the nanoscale. AFM is particularly advantageous for studying soft, semi-solid and heterogenous materials, such as biological samples, polymers and hydrogels in swollen state, because it can operate in various environments including air and liquid.

The force spectroscopy using AFM was employed for the study on mechanical properties at the nanoscale of semi-solid polysaccharide hydrogels, which is the technique especially valuable for revealing the information about the sample's stiffness, elasticity and/or adhesion properties in their native environments.

Despite the fact that the advantages of force spectroscopy prevail, there are also some limitations and disadvantages in the study of hydrogel systems: i.) Hydrogels are soft and highly deformable materials, unfortunately because of this the AFM sharp tip can easily indent or damage the hydrogel, leading toe measurements that may not accurately reflect the native properties, ii.) the interactions between the AFM tip and the surface of hydrogel can be complex. For instance, the AFM tip might stick to the hydrogel due to its high-water content, leading to artefacts in the force spectroscopy measurements, iii.) the sort, highly hydrated nature of hydrogels can cause the AFM tip to become contaminated with hydrogel material during scanning. This complicates the interpretation of force-distance curves and may leading to artifacts in the force measurements, iv.) the nature (i.e. the presence of pores as well as polymer chains) of hydrogel samples can cause the relatively poor repeatability of force spectroscopy measurements if the standard (sharp, pyramidal) tips are used.

Due to the above-mentioned disadvantages of force spectroscopy in standard mode (i.e. with standard geometries), we decided to perform a targeted tip modification leading to tips with tailored tips for the measurement of hydrogel systems. Commercial tipless silicon nitride cantilevers (NP-O10, Bruker) were functionalized by 10 mm melamine spheres. The success of the modification was tested by scanning electron microscopy (Fig. 1).

The applicability of the functionalized tips was tested on polysaccharide (agarose) hydrogels. The results suggest that using modified tips compared to commercial sharp tips (TESPA-V2) gives more reliable results with higher reproducibility.



Figure 1: Tipless silicon nitride cantilevers for tip functionalization (left), functionalized cantilever with large 10 µm spherical tip (right)

#### Acknowledgement

The authors would like to thank their colleagues at CEITEC institute, specifically the Nanobiotechnology Core Facility research group, for their help in solving experimental problems related to tip modification.

# PW36: Unveiling Hydrogel Microarchitecture: Correlating Macrorheology and Microscopy for Sustainable Material Design

Trudicova Monika<sup>1</sup>, Sedlacek Petr<sup>1</sup>, Smilek Jiri<sup>1</sup>, Pekar Miloslav<sup>1</sup>

<sup>1</sup> Brno University of Technology, Faculty of Chemistry, Purkynova 464/118, 612 00 Brno, Czech Republic, Email: xctrudicova@vutbr.cz

#### Keywords: hydrogels, rheology, scanning electron microscopy, atomic force microscopy

Hydrogels are defined as systems containing a threedimensional network of polymer chains filled with water, finding versatile applications in wound dressings, controlled drug release, and scaffolds for tissue engineering [1]. Mechanical properties of hydrogels are essential for these applications; therefore, it is important to be able to analytically characterize them and understand all possible variables that influence these properties. The macro-rheological behavior of these materials is closely linked to their internal architecture, with mesh size and bond strength between nodes playing crucial roles in understanding their viscoelastic characteristics.

This study focuses on semi-interpenetrating hydrogels consisting of physically crosslinked polyvinyl alcohol (PVAI), chemically crosslinked poly(hydroxyethyl methacrylate) (pHEMA), and sodium polystyrene sulfonate (PSS) acting as the interpenetrating component. Rheological tests involving amplitude sweep and frequency sweep tests were conducted to analyze their viscoelastic properties. The amplitude sweep test results (see Figure 1 for typical results) are utilized to determine the limit of the linear viscoelastic region (LVR), which indicates the range within which the structure of the samples is intact. Within the LVR region, we evaluated the values of G' and G", revealing the elastic and viscous, respectively, nature of the sample deformation behavior.

In addition, frequency sweep tests were conducted to describe the time-dependent behavior of the samples under non-destructive deformation. These tests provide crucial insights into the behavior and internal structure of polymers, as well as the long-term stability of dispersions. Using the data obtained, simple mathematical approaches were applied to calculate critical architectural parameters such as mesh size and crosslinking density [2]. These calculations allowed connecting the observed behavior of the hydrogels with their internal structure.



Figure 1: Typical results from amplitude sweep tests for PVAI hydrogels crosslinked with borax (0 PSS without and 1 PSS with 0.1 wt. % interpenetrating component).

To complement these rheological analyses, we used scanning electron microscopy (SEM) and atomic force microscopy (AFM) to study the internal structure of the hydrogels. This interdisciplinary approach allowed for a detailed understanding of how structural features influence mechanical properties. Despite providing different and distinct information about network size, each method revealed a consistent trend across the samples. Therefore, individual methods can offer valuable complementary insights into the structure of hydrogels on their own; however, to obtain a comprehensive understanding, it is necessary to combine these methods.

Linking the viscoelastic properties with the internal structure of hydrogels offers significant insights for designing and optimizing preparation of hydrogel materials. These insights are crucial for advanced uses of these materials in tissue engineering, drug delivery, and other medical fields. Understanding the relationship between the mechanical properties and internal structure of hydrogels is key to developing efficient hydrogelinvolving technologies.

#### References

- [1] N. Peppas, European Journal of Pharmaceutics and Biopharmaceutics 50 (2000) 27-46.
- L. Pescosolido, L. Feruglio, R. Farra, S. Fiorentino, I. Colombo, T. Coviello, P. Matricardi, W. Hennink, T. Vermonden, M. Grassi, Soft Matter 8 (2012) 7708-7715.

# PW37: UHPC Made with Recycled PET Fibers for the Improvement of Fire Resistance

**Bocian Luboš**<sup>1</sup>, Šoukal František<sup>1</sup>, Novotný Radoslav<sup>1</sup>, Sokola Patrik<sup>1</sup>, Markusík David<sup>1</sup>, Bubeník Jan<sup>2</sup>, Zach Jiří<sup>2</sup>, Novák Vítězslav<sup>2</sup>

- <sup>1</sup> Brno University of Technology, Faculty of Chemistry, Purkyňova 464/118, Brno, 612 00, email: xcbocian@vutbr.cz
- <sup>2</sup> Brno University of Technology, Faculty of Civil Engineering, Veveří 331/95, Brno, 602 00

Keywords: hybrid fiber reinforced concrete, high temperature performance, reactive powder concrete,

The hybrid fiber reinforced UHPC (ultra-high performance concrete) combines two types of fibers with different properties to obtain synergistic effect [1, 2]. These types of blends are often used for the enhancement of the resistance to high temperature and mechanical properties. However, mixtures of polyvinyl alcohol or polypropylene fibers with steel fibers are often being used for these types of studies. This means that there is lack of the research delving into the hybrid reinforcement of UHPC with the mixture of steel fibers and PET (polyethylene terephthalate) fibers made from recycled waste mainly on the resistance of UHPC to high temperature [3-5]. Thus, the high temperature resistance along with other properties of the UHPC reinforced with a mixture of steel and PET fibers is investigated in this study.

Two mixtures were made. One mixture contained 2.0 vol. % of steel fibers while the second mixture also contained 0.125 % of the PET fibers. The specimens with the dimensions of  $4 \times 4 \times 16$  cm were prepared for the testing of mechanical properties after 7, 14 and 28 days and the specimens with dimensions  $10 \times 5 \times 120$  cm were prepared for the testing of high temperature resistance after 28 days. The mini-cone slump flow test was conducted before the fabrication of the specimens.

The flexural and compressive strengths were then obtained according to the ISO 196-1 standard. The

maximum stress was also recorded in the case of the flexural strength. The testing of high temperature resistance was done by laying the specimens with the dimensions of  $10 \times 5 \times 120$  cm onto the furnace and the testing according to the standards EN 1363-1 and ISO 834 was conducted. Lastly, thin cross sections of composites before and after high temperature testing were cut and polished for BSEM (backscattered electron microscopy) imaging which mainly revealed the changes in microstructure caused by subjecting the specimens to high temperature.

The addition of the PET fibers contributed to significant decrease in slump flow which is thought to be the main limiting factor for addition of more PET fibers. Secondly, the addition of the PET fibers into the mixture had statistically negligible effect on the mechanical properties. However, the high temperature testing revealed that the addition of the PET fibers into the mixture significantly reduces spalling of the cementitious composites. Lastly, the BSEM imaging validated the contribution of the PET fibers for the increase in the high temperature resistance in terms of their melting away during the subjection of the specimens to high temperatures. It also revealed very dense matrix of manufactured concrete.

- [1] Z. Algin, M. Ozen, Construction and Building Materials (2018) 186.
- [2] J. Li, Z. Deng. Structural Concrete 1 (2023) 24.
- [3] S. Sanchayan, S.J. Foster, Materials and Structures 3 (2016) 49.
- [4] H. Li, G. Liu, International Journal of Concrete Structures and Materials 1 (2016) 10.
- [5] J.M. Irwan, R.M. Asyraf, N. Othman, K.H. Koh, M.M.K. Annas, S.K. Faisal, Advanced Materials Research (2013) 795.

#### Acknowledgement

References

This paper has been funded by project FAST/FCH-J-23-8248 "Development and study of behavior of UHPC with silanizated microfibers under extreme high temperature conditions".

### PW38: Photoactive Foil with Antibacterial Properties

#### Fanglová Michaela<sup>1</sup>, Veselý Michal<sup>1</sup>

<sup>1</sup> Brno University of Technology, Faculty of Chemistry, Purkynova 464/118, 612 00 Brno, Czech Republic, Email: Michaela.Fanglova@vut.cz

#### Keywords: photochemistry, photoactive foil, light, antibacterial properties

The Covid-19 epidemic has significantly increased our awareness of the risks associated with touching the various surfaces we encounter every day. Touch screens in shopping malls, fast food or airports have emerged as potentially dangerous sources of transmission of microorganisms, including bacteria and viruses. To reduce the risk of infection, special foil with antiviral and antibacterial properties have been installed on these screens. The low concentration of organic biocides and the effectiveness of photogenerated singlet oxygen make these foil not only effective but also safe for use in high human contact environments, which helps to protect public health.

The principle of the self-adhesive printed foil with antiviral and antimicrobial function is a combination of organic biocides and special photosensitive substances that use light energy to produce reactive oxygen species. The key component in this printed layer is zinc phthalocyanine, a substance activated by sunlight or visible light in the 600 to 700 nm. Zinc phthalocyanine absorbs light, causing it to be excited to the triplet state. In the excited triplet state, phthalocyanine interacts with molecular oxygen. This interaction leads to quenching of the triplet state of phthalocyanine and energy transfer to the oxygen molecules. The transfer of energy to oxygen leads to the formation of singlet oxygen, a powerful oxidizing agent that destroys viruses and bacteria.

The ability to produce singlet oxygen is an essential property of the prepared antibacterial foil. Therefore, to assess the antibacterial ability, it is crucial to develop a procedure to determine the rate of singlet oxygen production. Singlet oxygen is determined using the DPIBF indicator in hexane, where the loss of the indicator in solution is monitored using absorption spectra.



Figure 1: SmartCoater 17

The production of these self-adhesive printed films uses a SmartCoater coating machine with roll-to-roll and slot die application systems. These techniques enable the efficient and continuous application of thin printed layers with a thickness of 2 - 4 micrometers. The DektaXT contact profilometer with Vision 64 software is used to measure the thickness of these layers. The instrument enables accurate measurement of layer thickness at the micrometer level, which is important for production quality control and ensuring consistency of film properties.

#### Acknowledgement

This work was financially supported by the Technology Agency of the Czech Republic, project FW03010006.

## PW39: Optimization of Printing Clichés for Pad Printing

#### Filipi Denisa<sup>1</sup>, Šerík Matej<sup>1</sup>, Veselý Michal<sup>1</sup>

<sup>1</sup> Brno university of Technology Faculty of Chemistry, Czech Republic, Email: Denisa.Filipi@vut.cz

Keywords: Pad printing, cliché, material printing, fluorescent markers

Pad printing is one of the industry's most widely used printing methods. The method involves transferring an image from a printing mold (cliché) through a silicone stamp onto the surface to be printed. Its greatest advantage is the ability to print images on flat surfaces and surfaces of any shape. [1] Thanks to this versatility, pad printing is used for printing on advertising and gift items, as well as in many industries such as automotive, cosmetic, electrical, and medical. Because pad printing can be used on non-planar objects, it is ideal for printing with functional inks. For example, it is used for printing sensor layers on various types of substrates and for printing flexible electronics where thin and precise layers are required.

To achieve correct printing, choosing the right printing form is essential – a cliché that significantly impacts the final prints. The cliché determines the transferred motif's shape and thickness, which is crucial, especially when printing functional inks. To ensure the best printing properties, polymer, steel, and glass clichés were produced and their properties were studied. The goal of optimizing the printing clichés was to use them for printing fluorescent markers for polymer material selection.

The depth of the prepared clichés was determined by profilometry. Subsequently, prints of fluorescent markers using different clichés were compared in terms of the homogeneity and thickness of the prepared layers. The results of the profilometric measurement and the subsequent evaluation of print quality showed that fluorescent markers prepared using steel clichés exhibited the highest layer homogeneity.



Figure 1: Pad printing scheme [2]

#### References

[1] M. Kaplanová, Moderní polygrafie, Praha: Svaz polygrafických podnikatelů, 2009, p. 244–247.

[2] What is Pad Printing? Published July 17, 2018. Accessed June 28, 2024. https://artechpadprinting.com/padprinting/

#### Acknowledgement

This work was financially supported by the Technology Agency of the Czech Republic within the National Centres of Competence Programme – Polymers for the 21<sup>st</sup> Century.

# PW40: Kraft Lignin as Bio-Based Dielectric Polymer for Organic Field-Effect Transistors

**Cristian Vlad Irimia**<sup>1</sup>, Rosarita D'Oorsi<sup>2</sup>, Jeanette Lucejko<sup>2</sup>, Cigdem Yumusaki<sup>1</sup>, Niyazi Serdar Sariciftci<sup>1</sup>, Mihai Irimia-Vladu<sup>1</sup>, Alessandra Operamolla2

- <sup>1</sup> Johannes Kepler University Linz, Institute for Physical Chemistry, Linz Institute for Organic Solar Cells, TNF Tower, 8th floor, Altenberger Str. Nr. 69, 4040 Linz, Austria, Email: cristian.v.irimia@gmail.com
- <sup>2</sup> Dipartimento di Chimica e Chimica Industriale, Università di Pisa, Pisa, Italy

#### Keywords: Kraft lignin, natural dielectrics, nature-origin materials

The main focus of this work is the investigation of the dielectric layer, that is an essential component of field effect transistors. Despite the huge amount of yearly produced lignin waste, it finds scarce application as a fine material and is usually destined to be combusted in thermochemical plants to feed, with low efficiency, other industrial processes. So far, the use of lignin in materials science has been limited by the scarce knowledge of its molecular structure and properties, depending also on its isolation method. Lignin represents therefore an intriguing feedstock of organic material with immense availability, ranging between 50 to 80 million tons/year. In this work, we analyze the structural and chemical-physical characteristics of two kraft lignins and utilize them in the fabrication of organic field effect transistors.

As thin dielectric layer material for the aluminium gate electrode, two commercially available Kraft lignins (L1 and L2, both purchased from Sigma-Aldrich) were investigated. First, we apply several molecular characterization techniques, such as ATR-FTIR, elemental analyses, GPC-HPLC, EGA-MS, UV-Vis, 31P- and 13C-NMR spectroscopies to get insights into their different structures and their degree of molecular degradation. Then, we demonstrate their efficient application as gate dielectric materials for organic field-effect transistors (OFETs), finding the increased capacity of L1 with respect to L2 in triggering functional and efficient devices with both p-type and n-type organic semiconductor molecules [1].

The two dielectric materials investigated in this study are practical alternatives for the fabrication of sustainable, "green" electronics, considering their natural origin and wide availability, their low cost of production (they are with this respect simply a byproduct of paper and nanocellulose production), their low toxicity, inherent biocompatibility and biodegradability, and finally the most important aspect, their ultimate performance, and stabilityreliability in practical devices.

These lignin dielectrics show good film forming characteristics, high hydrophilicity, excellent dielectric behavior over a wide frequency range and good insulating properties in OFET devices operating at voltages as low as 1.5 V. Such dielectric materials may find their applicability in biodegradable devices operating at low voltages.

#### References

[1] R. D'Orsi, V. V. Irimia, J. J. Lucejko, B. Kahraman, Y. Kanbur, C. Yumusak, F. Babudri, M. Irimia Vladu, A. Operamolla, *Adv. Sust. Syst.* 6 (2022) 2200285.

#### Acknowledgement

Financial support from the project "EINSTEIN", grant number. 101136377 (HORIZON-WIDERA-2023-ACCESS-03) is gratefully acknowledged. We also gratefully acknowledge the Wittgenstein Prize of the Austrian Foundation of Advancement of Science (FWF) for Prof. Serdar Sariciftci (project number Z 222-N19).

# PW41: Preparation and Characterization of Layered Double Hydroxides on Mg Substrates Prepared by Powder Metallurgy

Kobzinková Eliška<sup>1</sup>, Buchtík Martin<sup>1</sup>, Březina Matěj<sup>1</sup>, Wasserbauer Jaromír<sup>1</sup>, Doskočil Leoš<sup>1</sup>

<sup>1</sup> Materials Research Centre, Faculty of Chemistry, Brno University of Technology, Purkyňova 464/118, 612 00 Brno, Czech Republic, Email: Eliska.Kobzinkova@vut.cz

Keywords: LDH coating, MgAl-LDH, magnesium, powder metallurgy, corrosion behavior, structural analysis.

This study deals with the preparation and characterization of layered double hydroxides (LDH) on Mg substrates prepared by powder metallurgy (PM). The work focuses on the optimization of the preparation of MgAl-LDH. Preparation conditions such as pH (10 and 12), temperature (90 and 100 °C) pressure and time were varied. In particular, the morphology and structure of the coatings and their elemental composition were evaluated. The evaluation was carried out using a scanning electron microscope (SEM) with an energy dispersive spectrometer (EDS). The optimized coatings were found to be uniform without defects with a thickness of 1 um. The electrochemical corrosion properties of the optimized MgAl-LDH coatings were also evaluated using potentiodynamic tests in a Hank's corrosion solution environment. Corrosion tests were shown to improve corrosion resistance, with a decrease in corrosion current density from  $58.8 \pm 2.5 \,\mu\text{A/cm}^2$  for uncoated PM Mg to  $1.1 \pm 0.4 \,\mu\text{A/cm}^2$ .

Magnesium and its alloys are suitable candidates for biomedical applications as biodegradable implants due to their high specific strength and elastic modulus similar to human bone. Their ability to degrade to form non-toxic products in biological systems also allows the use of Mg materials in medicine, especially in orthopedics for implants and stents [1].

One of the very progressive and applicable methods for the production of bioavailable materials with specific structures is the PM method. Moreover, the characteristic feature of materials prepared by PM is their porosity [2]. Porosity is advantageous for bioapplications because it allows the integration of e.g. bone tissue, smooth transport of fluids and drugs and also improves and implant tissue outgrowths in the healing process [1]. The present work deals with the possibility of preparing Mg corrosion protection using LDH based coatings. Layered double hydroxide based coatings have previously shown great potential for corrosion protection of magnesium alloys [3, 4].

The optimum preparation conditions were found to be 95 °C for 9 hours in 0.1 M Al(NO<sub>3</sub>)<sub>3</sub> solution at pH 10 under normal pressure. As can be seen in Fig. 1 the prepared coating is homogeneous in terms of morphology. A temperature of 100 °C and pH 12 proved unsuitable for coating formation. Shorter times do not produce a coating of sufficient thickness and higher times lead to degradation of the Mg substrate.



Fig. 1: Surface of optimized sample (SEM).

#### References

- [1] M. P. Staiger, A. M. Pietak, J. D. Huadmai, G. Dias, Biomaterials 9 (2006) 1728-1734.
- [2] S. Jaysathyakawin, M. Ravichandran, N. Baskar, C. Anand Chairman, R. Balasundaram, *Materials Today: Proceedings*, Part 2, (2020), 736-741.
- [3] Layered Double Hydroxide Polymer Nanocomposites, D. Saju, T. Sabu (Eds.), Woodhead Publishing, 2019.
- [4] F. Peng, H. Li, D. Wang, P. Tian, Y. Tian, ACS applied materials & interfaces 51 (2016), 35033-35044.

#### Acknowledgement

This work was supported by Specific University Research at FCH BUT, Project Nr. FCH-S-22-8012, Ministry of Education, Youth and Sports of the Czech Republic

# PW42: Comparative Study of the Effect of Lignosulfonate Plasticizer on Rheological Behaviour of Various Alkali-Activated Materials and Cement Pastes

#### Markusík David<sup>1</sup>, Bílek Vlastimil<sup>1</sup>

<sup>1</sup> Brno University of Technology, Faculty of Chemistry, Institute of Materials Chemistry; Purkyňova 464/118, 612 00 Brno, Czech Republic; Email: xcmarkusik@vutbr.cz

Keywords: lignosulfonate plasticizer, oscillatory measurements, flow point, amplitude sweep, plasticizing effect

Alkali-activated materials (AAMs) are more sustainable alternative to ordinary Portland cement binders in the construction and building industry. However, these materials come with some cons, namely poor workability along with the limited effectiveness of commercially available plasticizers are some of the main issues [1]. Therefore, this study deals with the effect of different doses of lignosulfonate (LS) plasticizer in AAMs on their rheological properties and was based on previous experiments by Kalina [2] and Bílek [3].

To prepare AAM pastes, commonly used alkaline activators with a concentration of Na+ 4 mol·dm<sup>-3</sup> and precursors, namely ground granulated blast furnace slag, low calcium fly-ash and metakaolin were used. The effectiveness of the LS plasticizer was also investigated in Portland cement-based pastes to compare the functionality in more known systems. The rheology was tested by rotation and oscillation measurements using a DHR-2 rheometer, where the results of the rotation measurements were analysed by the Herschel-Bulkley model, and the oscillation measurements were amplitude sweep tests with evaluation of yield point and flow point. LS showed a significant improvement on workability in pastes activated by NaOH, namely in slag pastes (Figure 1).



Figure 1: Influence of LS dose on complex modulus of studied NaOH-activated slag pastes

These rheological tests are also supported by plasticizer adsorption tests on the precursors used. LS also showed the marginal impact of rheology in metakaolinbased pastes, because rheology of MK-based geopolymers is primary influenced by viscosity of used alkaline activator [4].

#### References

- [1] J. L. Provis, Cement and Concrete Research 114 (2018), 40-48.
- [2] L. Kalina, V. Bílek, P. Hrubý, V. Iliushchenko, M. Kalina, J. Smilek, Cement and Concrete Research 157 (2022).
- [3] V. Bílek, L. Kalina, R. Novotný, Construction and Building Materials 386 (2023).
- [4] A. Favier, J. Hot, G. Habert, N. Roussel, J.-B. d'Espinose de Lacaillerie, Soft matter 1(8) (2014), 1134-1141.

# PW43: Design of Hollow Fiber Membrane Module for Membrane Distillation

#### Menshikh Maksim<sup>1</sup>

<sup>1</sup> Brno University of Technology, Faculty of Chemistry, Purkyňova 464/118, Brno, 612 00, Czech Republic, Email: Maksim.Menshikh@vut.cz

#### Keywords: Membranes, Membrane distillation, Hollow fibers.

This study presents the design and optimization of a hollow fiber membrane module tailored for membrane distillation (MD) applications. Membrane distillation is a thermally-driven separation process where a hydrophobic membrane facilitates the passage of water vapor while rejecting non-volatile solutes. The hollow fiber configuration offers several advantages, including high surface area-to-volume ratio and compact module design, which are crucial for enhancing the efficiency and scalability of MD systems. The research delves into various design parameters such as fiber material selection, pore size distribution, fiber packing density, and module configuration.

Computations of fluid dynamics (CFD) are employed to analyze the flow dynamics and heat transfer characteristics within the module, optimizing for maximum permeate flux and thermal efficiency. Experimental validation is conducted using a prototype module, and performance metrics such as water vapor flux, energy consumption, and salt rejection rate are evaluated.

The results are estimated to be that the optimized hollow fiber membrane module exhibits superior performance in terms of permeate flux and energy efficiency compared to traditional flat-sheet modules.

This work provides a comprehensive framework for the design and development of high-performance hollow fiber membrane modules for scalable and efficient membrane distillation systems.



Figure 1: 3D model of laboratory-scale hollow fiber membrane module

#### References

- [1] Membrane distillation based on polypropylene hollow fibers: development and testing of laboratory unit, B. Kalnická, Brno, Czechia, 2023.
- [2] Sharad Gupta, Industrial & Engineering Chemistry Research 26 (1987) 2323.
- [3] M. Doshi, V. Kabadi, AIChE Journal 23 (1977) 765.

#### Acknowledgement

Thanks to the Technology Agency of the Czech Republic, TREND programme № FW06010715

## **PW44: Thermal Properties of Selected Bio Phase Change Materials**

#### Řezáčová Veronika<sup>1</sup>, Ostrý Milan<sup>2</sup>

- <sup>1</sup> Institute of Chemistry and Technology of Environmental Protection, Faculty of Chemistry, Brno University of Technology, Purkyňova 118, 612 00 Brno, Email: rezacova@fch.vut.cz
- <sup>2</sup> Institute of Building Structures, Faculty of Civil Engineering, Brno University of Technology, Veveří 331/95, 602 00 Brno

#### Keywords: phase change materials (PCMs), coconut oil

Phase change materials (PCMs) refer to substances that can absorb or release thermal energy throughout the melting and freezing process.

PCMs are a very promising and useful tool in many areas of industry. For example, PCMs can serve as heat storage materials (for solar energy storage and accumulation), heat transfer media (for cooling, heating of buildings) or thermal protection in electronic devices. They can also be used in the medical, textile, food, automotive or chemical industries. The use of these materials can lead to energy savings, economic benefits as well as minimising the greenhouse effect.

PCMs are divided into three categories based on their composition. The first group includes organic PCMs. Organic PCMs are currently the most popular group of phase change materials. They are further divided into two subgroups, paraffinic (petroleum-based) and nonparaffinic (alcohols, ethers, glycols and fatty acid). This subgroup of non-paraffin PCMs also includes substances of natural origin called biobased PCMs (bio PCMs, BPCMs). These are materials obtained from a renewable, sustainable and environmentally friendly source. Such materials can come, for example, from the agri-food sector and its by-products such as palm kernel oil, palm oil, coconut oil or soybean oil. The second category of PCMs is inorganic PCMs (hydrated salts, alloys, metals). The third category is eutectic PCMs, they are divided according to the origin of the components into: organic-organic, inorganic-inorganic or inorganic-organic [1-2].

Our work is focused on analysis of the basic thermal properties of selected natural materials with phase transformation heat accumulation potential (bio PCMs) and the subsequent detailed characterization of materials suitable for construction industry applications.

#### References

- [1] H. Mehling, M. Brütting, T. Haussmann, *Nature* 20 (2001) 537.
- [2] K. Pielichowska, K. Nowicka-Dunal, K. Pielichowski, Polymers 16 (2024), 328.
- [3] M. Ostrý, S. Bantová, V. Řezáčová, SSP Journal of civil engineering 17 (2022) 1.

#### Acknowledgement

The work was supported by the project FCH-S-24-8591 of Ministry of Education, Youth and Sports of the Czech Republic.

The thermal properties of the selected PCMs were monitored by a differential compensation calorimeter DSC 2500 from TA Instruments. Trios software was used to control it and evaluate the results. A total of 23 samples were analysed, specifically different types of oils, bee products (wax, propolis) and animal fats.

The measured data show that many vegetable oils have a monitored phase transition at temperatures below 0°C. These bio PCMs have the potential to be used in cooling systems. In contrast, the measured bee products have phase transition temperatures above 60°C. Coconut oil was evaluated as a material suitable for applications in the construction industry with melting temperature 22,6°C (see Fig. 1). The response on different temperature treatment and time stability tests were performed with satisfactory results for practical applications [3].



Figure 1: DSC record of coconut oil (Purity Vision, Natures Care CZ)

# PW45: Valorization of Hemp Processing Byproducts for Innovative Cosmetic Applications

Monika Wikarska<sup>1</sup>, Darina Kohútová<sup>1</sup>, Sarah Benková<sup>1</sup>, Lenka Gregarová<sup>1</sup>, Ivana Márová<sup>1</sup>

<sup>1</sup> Brno University of Technology, Faculty of Chemistry, Purkyňova 464/118, 612 00 Brno, Email: xcwikarska@vutbr.cz

#### Keywords: hempseed meal, valorization, cosmetics, sustainability

The sustainable utilization of agricultural byproducts is essential for promoting eco-friendly practices across various industries. Hemp processing generates a range of byproducts that can be valorized to enhance both sustainability and economic value.

This study explores the valorization of byproducts from hemp (*Cannabis sativa L.*) processing, focusing on their potential applications in the cosmetic sector (shown in Figure 1). The studied hemp breeds were cultivated primarily for the production of hemp oil and cannabinoid extract. The processing of hemp involves multiple stages, each producing distinct byproducts. We examined three of these byproducts, rich in proteins, sugars, and lipids (Table 1). Hemp seed meal (HSM) and hemp sludge (HS) from cold-pressing seeds for oil extraction, and residual biomass (BAE) from the ethanol extraction of cannabinoids from inflorescences and leaves offer diverse opportunities for further utilization in cosmetic applications.

HSM, rich in proteins, sugars, and residual oil [1], was subjected to hydrothermal extraction and enzymatic hydrolysis to extract water-soluble proteins for haircare formulations, enhancing their nutritive and conditioning properties. This process yielded hemp protein hydrolysate (HPH), a mixture of polypeptides, oligopeptides, and amino acids known for their numerous biological activities [2]. We incorporated HPH into shampoo and conditioner formulations to improve hair reparation due to its soluble proteins and moisturizing effects. Additionally, all the byproducts, HSM, HS, and BAE, were used for the fermentation of the red yeast Rhodosporidium toruloides. This fermentation yielded a ferment containing bioactive compounds such as coenzyme Q10, lipids, carotenoids, and vitamin E, each substrate resulting in a different composition of bioactive compounds.

*R. toruloides* is a non-conventional, oleaginous yeast with a natural carotenoid pathway that accumulates high lipid content. Its lipid extract has demonstrated the ability to increase filaggrin expression, suppress MMP-1 expression under heat stress in keratinocytes, and exhibit

antioxidation activity as confirmed by the DPPH assay, highlighting its potential for cosmetic applications [3].

Moreover, hempseed sludge was repurposed for soap production, utilizing its lipid content to create moisturizing soaps with great foamability and exfoliating effects – broadening the industrial application of this waste material.

Byproduct of Hemp Precessing	Protein content	Sugar content	Lipid content
Hemp seed meal (HPH)	15,6 ± 1,1 %	7,2 ± 0,6 %	3,4 ± 0,2 %
Hemp sludge (HS)	0,8±0,1%	4,8 ± 0,6 %	39,2 ±1,5 %
Biomass after extraction (BAE)	13,3 ± 0,9 %	15,2 ± 1,1 %	0,7 ± 1,0 %

Table 1: Nutritional Composition of Byproducts from Hemp Processing

This research highlights the significant potential of hemp processing byproducts as valuable resources for creating high-performance, sustainable cosmetics. Our findings contribute to waste reduction and add economic value to the hemp industry, promoting a more sustainable and circular economy.



Figure 1: Schematic Abstract of Utilization of Hemp Byproducts for Cosmetic Applications

#### References

- [1] M. Pojić, A. Mišan, M. Sakač, Journal of Agricultural and Food Chemistry, 62 (2014), 12436–12442
- [2] G. Aiello, C. Lammi, G. Boschin, Journal of Agricultural and Food Chemistry 65 (2017) 10174–10184
- [3] J. Kim, E.-J. Lee, K.-E. Lee, Computational and Structural Biotechnology Journal 21 (2023) 2009-2017

#### Acknowledgement

This research was funded by FCH-S-24-8526 of Faculty of Chemistry.

# PO1: Synthesis and Electrochemical Characterization of New Semiconductive Materials with Amino Acid Side Chain for Bioelectronics

Arkhiptsava Katsiaryna<sup>1</sup>, Richtár Jan<sup>1</sup>, Kousseff Christina<sup>2</sup>, Krajčovič Jozef<sup>1</sup>

- 1 Brno University of Technology, Faculty of Chemistry, Purkyňova 464/118, 612 00 Brno, Czech Republic, Email: Katsiaryna.Arkhiptsava@vut.cz
- 2 University of Oxford, 12 Mansfield Road, Oxford OX1 3TA, United Kingdom

#### Keywords: semiconductors, polymers, organic chemistry

Bioelectronics is a rapidly advancing field that bridges the gap between biological systems and electronic signals. This interdisciplinary domain focuses on the development of devices capable of converting and interpreting signals from biological entities [1]. These technologies have vast applications in medicine, sensors, and health monitoring devices.

Among the various organic electronic devices, organic electrochemical transistors (OECTs) stand out due to their ability to amplify weak electrical signals, high sensitivity, cost-effectiveness, ease of operation, and compatibility with flexible and wearable devices [2]. The active channel of OECTs often consists of organic polymers with conjugated  $\pi$ -systems and mixed ion-electron conductivity, which allows for direct interaction with biological samples. This makes the increasing of biocompatibility of active channel desirable. However, current materials often suffer from drawbacks such as low conductivity, sensitivity, stability, and biocompatibility. Overcoming these limitations requires innovative molecular design and the development of selective and efficient synthetic methodologies.

This study focuses on the synthesis of a series of semiconductive polymers and copolymers featuring novel

#### References

- [1] Y. He, N. A. Kukhta, A. Marks, and C. K. Luscombe, Journal of Materials Chemistry C 10 (2022) 2314-2332.
- [2] Z. Zhao, Z. Tian, and F. Yan, Cell Reports Physical Science. 4 (2023) 101673.

#### Acknowledgement

The authors thank the projects FCH-S-23-8208 and Aktion (MŠMT) No. 95p3, The Faculty of Chemistry BUT for providing the facilities for the study.

bioinspired side chains. The side chains of the synthesized polymers incorporate amino acids, which are linked to the main chain via glycol linkers of varying lengths. This design aims to enhance the properties of the materials, making them more suitable for bioelectronic applications. In this presentation the synthesis and studying of electrochemical properties are discussed.



Figure 1: Common structure of synthesized semiconductive copolymers

# PO2: Organic Electrochemical Transistor as a Device for Studying Electrical Properties of Smart Ionic Liquids

**Blahut Jan**<sup>1</sup>, Svoboda Petr<sup>2</sup>, Michalec Michal<sup>2</sup>, Foltýn Jan<sup>2</sup>, Schneider David<sup>2</sup>, Menčík Přemysl<sup>1</sup>, Zmeškal Oldřich<sup>1</sup>

- <sup>1</sup> Faculty of Chemistry, Institute of Physical and Applied Chemistry, Purkyňova 464/118, Brno, Czech Republic, Email: Jan.Blahut@vutbr.cz
- <sup>2</sup> Faculty of Mechanical Engineering, Institute of Machine and Industrial Design, Technická 2896/2, Brno, Czech Republic

Keywords: Ionic liquid, OECT, SCLC, tribology, PLA, [EMIM][Tf2N], [BMIM][SO<sub>3</sub>CF<sub>3</sub>]

lonic liquids (ILs) represent an innovative alternative to traditional synthetic oils used as lubricants in the field of tribology. These liquids are defined by their ability to exist in a liquid state at temperatures below 100 °C. ILs have several unique properties that make them "smart liquids" and ideal for use in tribological applications [1].

One of the main reasons why ILs are considered smart fluids is their ability to change rheological and tribological properties in response to external stimuli such as light, heat, magnetic or electric fields. This adaptability enables precise control of their performance in different operating conditions. ILs also have very low vapor pressure, high thermal stability and low volatility, which means they can safely operate in extreme temperature and pressure conditions without the risk of vaporization or ignition [2].

Another significant advantage of ILs is their ecological potential. Since they do not contain volatile organic compounds, they minimize the risk of environmental pollution. This makes them an attractive alternative to traditional lubricants, which often contain harmful chemicals. ILs also show an excellent ability to reduce friction and wear, thereby extending the life of machinery and reducing maintenance and repair costs [3].

Moreover, due to their chemical variability, ILs can be designed to meet the specific requirements of different applications. This includes optimizing their compatibility with different materials and ensuring maximum performance in specific operating conditions.

This study is focused on determination and analysis of electrical properties of two ionic liquids ([EMIM][Tf2N],  $[BMIM][SO_3CF_3]$ , *Figure 1*) by using a PLA organic electrochemical transistor (OECT) device. The ability to manipulate ions by applying the external electric field was determined by measuring the volt-ampere characteristics. This study is necessary to thoroughly study and reliably describe the mechanism of influencing the rheological and tribological properties of these smart liquids by an external electric field.



Figure 1: Studied ILs. [EMIM][Tf2N] (left) and  $[BMIM][SO_3CF_3]$  (right).

The OECT consists of three electrodes. Source, drain and gate. A  $U_{SD}$  voltage was applied between the source and drain electrodes, a second  $U_{GD}$  voltage was applied between the gate and drain electrodes. The  $I_{SD}$  current flowing through the semiconductor channel between source and drain electrodes was influenced by changing the value of  $U_{GD}$  voltage.



Figure 2: Volt-ampere characteristics of [EMIM][Tf2N] (red) and [BMIM][SO<sub>3</sub>CF<sub>3</sub>] (yellow).

#### References

- [1] M. Cai, Q. Yu, W. Liu, F. Zhou, Chemical Society Reviews 49(21) (2020) 7753-7818.
- [2] I. Minami, Molecules 14(6) (2009) 2286-2305.
- [3] M. Michalec, P. Svoboda, I. Krupka, M. Hartl, Tribology in Industry 40(4) (2018) 515-528.

#### Acknowledgement

J. Blahut acknowledges financial support from Interfaculty project FCH/FSI-J-24-8501.

# PO3: Thionation of Lactam-Containing Organic Pigments as a Synthetic Tool for Near-Infrared Absorbing n-Type Semiconductors

Cigánek Martin<sup>1</sup>, Kratochvíl Matouš<sup>1</sup>, Yumusak Cigdem<sup>2</sup>, Sariciftci Niyazi Serdar<sup>2</sup>, Krajčovič Jozef<sup>1</sup>

- <sup>1</sup> Brno University of Technology, Faculty of Chemistry, Purkyňova 118, 612 00 Brno, Czech Republic, Email: martin.ciganek@fch.vut.cz
- <sup>2</sup> Johannes Kepler University Linz, Linz Institute for Organic Solar Cells (LIOS), Physical Chemistry, Altenbergerstraße 69, 4040 Linz, Austria

Keywords: organic photovoltaics, hydrogen-bonded pigments, diketopyrrolopyrrole, n-type semiconductors

The diketopyrrolopyrrole derivatives (DPPs) belong to the major organic high-performance pigments finding several significant applications in diverse areas of organic electronics [1]. The core of these derivatives is formed by a molecule with the systematic name 2,5-dihydropyrrolo[4,3-c]pyrrolo-1,4-dione, which offers a wide range of possible structural modifications. One of the important derivatisations is the conversion of oxygen atoms in keto groups to sulfur atoms *via* one-step thionation using Lawesson's reagent [2]. In this work, basic thiophenyl (**Th-DPP**) and phenyl (**Ph-DPP**) DPP molecules were used as starting materials for the preparation of sulfur analogues **Th-DTPP** and **Ph-DTPP** (*Figure 1*), which were subsequently subjected to a study of electronic structure, optical and semiconducting properties.

Thionation brought a bathochromic shift of the solidstate absorption edge. Furthermore, the electronic structure of the studied DTPPs showed low-lying, highly stabilised LUMO orbitals (-4.5 eV), which was in good agreement with model calculations, whereas the experimental HOMO destabilisation was significantly higher than predicted (-5.6 eV). Finally, field effect mobilities were determined on a bottom-gate top-contact transistor, where thionation caused the switching of the ptype character of DPPs to the n-type character of DTPPs (*Table 1*) [3]. Since DTPPs are still sufficiently thermally stable and have near-infrared absorption capability, lowlying LUMO and n-type mobility, they can be considered potential electron-accepting components in photovoltaics.

In addition, a huge advantage is that derivatization by the thionation method represents a versatile tool for the conversion of a diverse range of organic pigments containing keto groups into their sulfur analogues.



Figure 1: Chemical structures of the studied organic pigments

Table 1. Field offect weakilities of the studied weaterials

Table 1: Field effect mobilities of the studied materials							
Contact material	Mobility	Th-DPP	Th-DTPP	Ph-DPP	Ph-DTPP		
AI [cm <sup>2</sup> ·V <sup>-1</sup> ·s <sup>-1</sup> ]	μе	1.2·10 <sup>-5</sup>	7.4·10 <sup>-3</sup>	2.7·10 <sup>-3</sup>	1.8·10 <sup>-2</sup>		
Au [cm <sup>2</sup> ·V <sup>-1</sup> ·s <sup>-1</sup> ]	μh	2.0·10 <sup>-3</sup>	4.9.10-4	6.6·10 <sup>-3</sup>	3.0.10-4		

#### References

- [1] M. Cigánek, J. Richtár, M. Weiter, J. Krajčovič, Isr. J. Chem. 61 (2021) 1-15.
- [2] F. Closs, R. Gompper, Angew. Chem. Int. Ed. Engl. 26 (1987) 552-554.
- [3] M. Kratochvíl, M. Cigánek, C. Yumusak et al., Dyes Pigm. 197 (2022) 109884.

#### Acknowledgement

The authors thank for their financial support the Ministry of Industry and Trade TRIO (project **No. FV20022**), the Czech Science Foundation grant No. **19-22783S** and Austrian Agency for International Cooperation in Education and Research (OEAD-GmbH, WTZ, CZ01/2020, **8J20AT025**).

# PO4: Use of Polyhydroxyalkanoates for Preparation of 3D Printable Hydrogels

Cernekova Nicole<sup>1</sup>, Kadlecova Zuzana<sup>2</sup>, Sedlacek Petr<sup>3</sup>, Smilek Jiri<sup>3</sup>, Vojtova Lucy<sup>2</sup>, Kovalcik Adriana<sup>1</sup>

- <sup>1</sup> Brno University of Technology, Faculty of Chemistry, Institute of Food Science and Biotechnology, Purkynova 464/118, 612 00 Brno, Czech Republic, Email: xccernekova@vutbr.cz
- <sup>2</sup> Brno University of Technology, Central European Research Institute, Purkynova 656/123, 621 00
  Brno, Czech Republic
- <sup>3</sup> Brno University of Technology, Faculty of Chemistry, Institute of Physical and Applied Chemistry, Purkynova 464/118, 612 00 Brno, Czech Republic

#### Keywords: 3D printing, polyhydroxyalkanoates, hydrogels

Hydrogels are an interesting and significant class of materials with diverse applications in several fields of biomedical field. Their prominence is continuously growing due to their unique properties dependent on the nature of the (bio)polymer from which they are prepared. In the most cases, hydrogels are composed of a hydrophilic cross-linked polymer permeating the entire dispersion medium (water). As well as their mechanical properties, these materials have a structure similar to the macromolecular composition of the human body's tissues. For this as one of many reasons, their research has led to the development of the new hydrogel materials for biomedicine, such as scaffolds or implants [1].

Various biomaterials and manufacturing methods, including 3D printing, have emerged to produce patient-specific bioactive scaffolds. Additive manufacturing has become a popular technology for fabricating implants with the potential to heal critical-sized defects [2]. Moreover, the geometry of the implants can be tailored to meet patient-specific defect needs.

Focusing on tissue engineering, polyhydroxyalkanoates (PHAs) have attracted considerable interest in the biomedical industry [3]. As intracellular biopolyesters produced by various microorganisms, they possess several valuable properties. These include biodegradability, biocompatibility and wide range of mechanical properties that are due to the diversity of PHAs. Since the final mechanical properties of hydrogels depend on their (bio)polymeric material, PHAs seem to be a very suitable source for their use in tissue engineering [4].

The main limitation of using PHAs in hydrogel chemistry is their hydrophobic nature, which is incompatible with hydrogel principles. Herein, we overcame this limitation using a solvent-exchange method. This method involves dissolving the polymer in a suitable water miscible solvent, such as DMSO or acetic acid [5], and then exchanging the solvent with water to form hydrogels. We designed hydrogels based on different types of PHAs and with the incorporation of additives. The effect of varying the composition, solvent or solventexchange method on mechanical properties of hydrogels has been compared. The use of PHAs in 3D printing of hydrogels has been described as well.

#### References

- [1] J. Li, et al., Front Bioengineering and Biotechnology 9 (2021), 763031.
- [2] B. Bisht, et al., Annals of Biomedical Engineering 49 (2021), 1128-50.
- [3] V. Kalia, et al., Polymers 15 (2023), 1937.
- [4] W. Guo, et al., Engineered Regeneration 3 (2022), 24-40.
- [5] P. Anbukarasu, et al., Scientific Reports 5 (2016), 17884.

#### Acknowledgement

The presented work was supported through the internal Brno University of Technology projects FCH-S-24-8526 and CEITEC VUT/FCH-J-24-8589.

#### Stevan Gavranovic<sup>1</sup>

<sup>1</sup> Brno University of Technology, Faculty of Chemistry, Materials Research Centre, Purkynova 118, 612 00 Brno, Czech Republic, Email: Stevan.Gavranovic@vut.cz

#### Keywords: additive technology, printed touch sensors, flexible electronics

It is nearly impossible to imagine a modern multifunctional electronic device without a touch screen. It became a preferred feature in both big (interactive kiosks, monitors, tablets, etc.) and small devices (smartphones, smart watches, controllers, etc.). Touch screens consist of an array of sensors that can detect touch input from a user. In this way, users interact directly with the displayed items and intuitively operate the device. Resistive and capacitive touchscreens are two main technologies used in a wide range of electronic devices.

In the resistive touch sensor, the touch is detected when a flexible, transparent top electrode makes a contact with the rigid bottom electrode. The contact can be creative with conductive (finger, stylus) or nonconductive object (through gloves, etc.). Thus, this technology is mainly used in the applications, where durability and precision are more important than the high sensitivity (i.e. industrial applications).

In contrast, the capacitive touchscreen detects touch when a conductive object (finger or stylus) alters the electrical field created by the electrodes inside the screen. In simpler capacitive systems, each electrode is connected to an individual sensor circuit. Once touched, the capacitance of a specific electrode increases, and the system detects this change. In more advanced systems (projected capacitive touch), the horizontal and vertical array of electrodes create a grid with uniform distribution of electric field. The screen controller scans each electrode intersection and detects the change of capacitance, allowing for precise detection. This type of touch screen supports multitouch and is generally more implemented in smartphones and tablets, due to the more user-friendly features.

The design of capacitive touch sensors and screens requires several key steps, combining material science and precision engineering: (i) material selection, (ii) design of electrode pattern, (iii) conductive layer coating, (iv) layer lamination, and (v) integration with display and final assembly.

The selection of conductive material and substrates depends on the desired properties of the touchscreen (sensor). Indium-tin oxide, aluminum-doped zinc oxide, and fluorine-doped tin oxides are typically used in highly

#### References

[1] T. Gray, Springer International Publishing, 2019.

#### Acknowledgement

The author acknowledges financial support from the Technological Agency of the Czech Republic through the National Competence Centres Programme, project No. TN02000067/008.

transparent touch screens for mobile devices. In contrast, wire mesh might be considered for screens with a lower demand for transparency. For flexible screens, one might consider plastic substrates, such as PET, or glass substrates.



Figure 1: Key steps in the design of capacitive touch sensor

New trends in touchscreen technology prefer implementation of silver nanowires and nonmetallic materials because of the lower cost and easier layer deposition. The nontransparent contact electrodes (i.e. perimeter traces) are typically made from silver paste.

The electrode pattern is the geometric orientation of the electrodes, typically a confidential design created to fit a specific application. The following steps are associated with the fabrication of the devices. Techniques such as sputtering, screen printing, laser etching, and lamination are used to produce touch sensors and touchscreens.

This poster will present the key steps in the design of capacitive touch sensors implemented in the project currently ongoing at the Faculty of Chemistry (FCH) of the Brno University of Technology (BUT). Each step will be presented and evaluated with respect to modern trends in touch technology. The unique approach applied at the FCH BUT will emphasize the use of novel materials to maximize performance and minimize the production costs of next-generation touchscreens.

#### Stevan Gavranovic<sup>1</sup>

<sup>1</sup> Brno University of Technology, Faculty of Chemistry, Materials Research Centre, Purkynova 118, 612 00 Brno, Czech Republic, Email: Stevan.Gavranovic@vut.cz

#### Keywords: touch technology, printed electronics, flexible sensor

This poster will evaluate two technologies commonly used for fabrication of touchscreens: (i) additive and (ii) subtractive technology. Additive technology involves building up or depositing materials layer by layer to create touchscreens with the desired electrode pattern and structure. On the contrary, subtractive technology typically involves subtracting material (pattering by laser etching or photolitography) from a conductive layer to create the required patterns and structures.

Modern touchscreens come in a broad variety of structures. With respect to the number of transparent conductive layers, we distinguish three different structures: (i) a single layered structure made of indium tin oxide (ITO) or similar material, applied to the substrate, usually glass or film, (ii) a double-layered structure made of two transparent conductive layers, often separated by an insulating layer, and (iii) a multilayered structure where more than two transparent conductive layers are used. The single-layered structure is thinner, lighter, and typically used in devices which support single-touch or basic multitouch, where high sensitivity is not required. In contrast, a double-layered and multi-layered structure is used for fabrication of touchscreens with extremely accurate touch detection and multitouch functionality. Nevertheless, adding layers of transparent conductive material increases the weight and the overall price of the devices.



Figure 1: a) comparison of additive and subtractive technology approaches

#### References

[1] T. Gray, Springer International Publishing, 2019

#### Acknowledgement

The author acknowledges financial support from the Technological Agency of the Czech Republic through the TACR National Competence Centres Programme, project No. TN02000067/008.

Modern trends in touch technology include the substitution of conventionally used materials such as indium tin oxide or aluminum-doped zinc oxide with silver nanowires or graphene. In addition to that, there is a great movement to utilize production to reach minimum material waste and maximize production efficiency.

The fabrication of the touchscreen usually has to take multiple steps: (i) material selection, (ii) design of the electrode pattern, (iii) conductive layer coating, (iv) layer lamination, and (v) integration with the display and final assembly.

Coating of the conductive material can be done with different techniques. The most commonly used tecniques are sputtering, chemical vapor deposition, and printing techniques (mainly screen printing or inkjet). Of the mention tecniques, only printing tecniques have the possibility to pattern during coating. Other techniques require patterning of the coated film either by polylitography or laser etching. This additional step generates non-reusable material waste that could increase the cost of production and decrease production efficiency. Moreover, laser ablation processes that are typically used in high-scale production are significantly slower than screen printing. However, unlike screen printing, laser etching can create a more precise structure with a shorter electrode distance, which increases the sensitivity of the sensor. In addition to that, change of the electrode pattern it is significantly easier than in screen printing.

This poster will evaluate both additive (screen printing) and subtractive (laser patterning) touch technologies in terms of material waste, speed, and accuracy of the final products. The additive touch technology applied in ongoing project at the Faculty of Chemistry will be presented in detail.

## PO7: Glass Microfluidics for Planar Lipid Bilayer Formation

#### Gjevik Alzbeta<sup>1,2</sup>, Sery Mojmir<sup>2</sup>, Pekar Miloslav<sup>1</sup>

- <sup>1</sup> Faculty of Chemistry, Brno University of Technology, Institute of Physical and Applied Chemistry, Purkyňova 464/118, 612 00 Brno, Czech Republic, Email: xcvargova@vutbr.cz
- <sup>2</sup> Institute of Scientific Instruments of the CAS, v.v.i., Department of Microphotonics, Kralovopolska 147, 612 00 Brno, Czech Republic

#### Keywords: microfluidics, glass chip, phospholipid bilayer, PLB, reactive ion etching, RIE,

Microfluidics is a field of research that studies how fluids move through sub millimeter spaces and that develops microscale fluid-processing technology [1].

Manipulation of liquids moving through micro-sized channels and ducts showcases their unique behaviors and has a wide range of applications across various fields, including medical diagnostics, biotechnology, food and environmental sciences. The prime examples are organon-chip, lab-on-chip and biosensor devices and droplet, emulsion and bubble generation devices. Our research area is cellular membrane model preparation on microfluidics with a focus on free-standing planar lipid bilayers.

Membrane models are a versatile tool for understanding the fundamental mechanisms of cellular function. Their applications range from the modeling of complex biological processes and protein characterization to the development of biosensors and drug delivery systems.

One of the most common ways of preparing microfluidic devices is photolithography for master mold fabrication followed by soft lithography (replica molding) of polydimethylsiloxane (PDMS) and bonding PDMS to glass with plasma treatment [2]. Although relatively fast and inexpensive, this technique is not particularly sustainable as it creates one time use devices. For this reason, we set out to create a reusable device made of glass.

Hence, this work summarizes means of glass microfluidic device fabrication and phospholipid bilayer formation mechanisms.

It showcases the design and preparation of a glass microfluidic chip and presents a microfluidic device prepared by lithography techniques and reactive ion etching, adapted for model membrane formation by selfassembly of phospholipids at the interface of aqueous and

#### References

- [1] G. M. Whitesides, Nature 442, 368–373 (2006)
- [2] A. G. Niculescu, C. Chircov, A. C. Bîrcă, A. M. Grumezescu, Int. J. Mol. Sci. (2021), 22, 2011
- [3] A. Gjevik, F. Mravec, M. Pekař, M. Šerý, V. Richterová, 21st IUVSTA Summer School on Physics at Nanoscale Book of Abstracts, Skalský dvůr, Czechia, 2024, p. 31

#### Acknowledgement

This work has been supported by Brno University of Technology Specific Research, project No. FCH-S-24-8568, by the Czech Academy of Sciences (RVO: 68081731) and the Technology Agency of the Czech Republic in the frame of the National Centres of Competence (TN02000020/Centre of Advanced Electron and Photonic Optics).

organic phases created by the architecture of the microfluidic device.

This device was previously fabricated out of PDMS and tested for functionality [3]. Glass also offers structural and optical benefits over PDMS.







Figure 2: Schema of membrane formation by selfassembly of phospholipids at the interface of aqueous and organic phase

# PO8: Testing the Antimicrobial Activity of Photocatalytic Surfaces Using Resazurin Assay

Králová Marcela<sup>1</sup>, Patakyová Sylvia<sup>1</sup>, Veselá Mária<sup>1</sup>, Veselý Michal<sup>1</sup>, Dzik Petr<sup>1</sup>

<sup>1</sup> Brno University of Technology, Faculty of Chemistry, Purkyňova 464/118, 612 00 Brno, Czech Republic, Email: kralova@fch.vut.cz

#### Keywords: resazurin assay, antimicrobial activity, photocatalytic surfaces

The antimicrobial activity of photocatalytic surfaces was tested using a resazurin assay. Resazurin is a blue, water-soluble compound that exhibits a weak degree of red fluorescence which gives a concentrated solution a purple tint. Upon reduction, associated with, for example, cellular respiration, resazurin is converted to resorufin (figure 1), a bright pink intermediate that emits an intensive orange fluorescence ( $\lambda max = 590 \text{ nm}$ ). This change is irreversible. In the second stage of reduction, the solution becomes completely colourless; this stage is reversible by the addition of atmospheric oxygen.[1] Resazurin is a substance that is very stable in a medium that contains no cells, but in the presence of viable cells it is very rapidly reduced to resorufin.[2]



Figure 1: Reduction of blue resazurin to pink resorufin and consequent change to colourless dihydroresorufin

The gram-negative bacteria *Escherichia coli* was chosen as the model microorganism. A bacteria inoculum with a concentration of  $1.75 \times 10^6$  CFU/ml was applied to hydrogel carriers and these were subsequently placed on the study surfaces. Half of the samples were kept in the dark and the other half were illuminated (900 lx). The study was carried out for three types of photocatalytic surfaces with the addition of different amounts of biocidal agent (D0, D50 and D200). After 4 hours, the carriers were transferred to vials, resazurin added and the number of viable cells in the mixture evaluated.

The time to reach maximum fluorescence (Figure 2) for each sample was recorded and the logarithm of the number of viable cells per cm<sup>2</sup> was calculated. The various parameters for the calculation were defined as: log  $C_L$  is photocatalytic surface under illumination, log  $C_D$  is the photocatalytic surface in the dark, log  $B_L$  is the blank under illumination, and log  $B_D$  is the blank in the dark. A summary of the average values can be found in Table 1. We can see that the number of viable cells in the illuminated samples decreased for all surface treatments, D0, D50, and D200. The authors observed that as the amount of biocide in the layer increased, the proportion of viable cells in the final antimicrobial activity of the samples is calculated according to the relationship:

$$\Delta R = \log(B_L/C_L) - \log(B_D/C_D) = R_L - R_D$$



Figure 2: Time at which maximum fluorescence was reached

Sample	D0	D50	D200
log C <sub>0</sub>	4.01	4.40	3.62
log C∟	2.97	3.66	2.83
log BL	3.90	4.25	3.86
RL	0.93	0.59	1.03
log C <sub>D</sub>	3.77	3.91	2.76
log B <sub>D</sub>	3.81	4.26	3.67
R <sub>D</sub>	0.04	0.35	0.91
ΔR	0.89	0.24	0.12

#### References

- [1] G. Jackson, H. Beyenal, W.M. Rees, Z. Lewandowski, J. of Microbiological Methods 47 (2001) 1-10.
- [2] E.Travnickova, P.Mikula, J.Oprsal, M.Bohacova, L.Kubac, D.Kimmer, J. Soukupova, M. Bittner, Amb Express 9 (2019).

#### Acknowledgement

This work was supported by the Czech Technology Agency through project: CZ.01.01.01/01/22\_002/0000322.

# PO9: Indigo Derivatives for Applications in Thin Film Organic Electronics

**Kratochvil Matous**<sup>1</sup>, Kumar Chandan<sup>2</sup>, Sanke Devendra<sup>2</sup>, Yumusak Cigdem<sup>3</sup>, Weiter Martin<sup>1</sup>, Zade Sanjio<sup>2</sup>

- <sup>1</sup> Brno University of Technology, Faculty of Chemistry, Materials Research Centre, Purkyňova 118, 612 00 Brno, Czech Republic, Email: Matous.Kratochvil@vubtr.cz
- <sup>2</sup> Department of Chemical Sciences and Centre for Advanced Functional Materials, Indian Institute of Science Education and Research (IISER) Kolkata, Mohanpur, Nadia 741246, West Bengal, India.
- <sup>3</sup> Linz Institute for Organic Solar Cells (LIOS), Physical Chemistry, Johannes Kepler University Linz, Altenbergerstraße 69, 4040 Linz, Austria.

Keywords: Indigo, Organic field-effect transistors (OFET), p-type, n-type, Ambipolar, Hole mobility, electron mobility

The development of organic electronics had seen the research focus on well-known organic pigments and dyes. One of these was indigo and its derivatives. The identification of indigo's semiconducting properties [1-4] have sparked a renewed interest in indigo chemistry. The functionalization has been used as a tool to fine tune the properties of novel materials. Indigo is an organic pigment with very poor solubility. This drawback may be overcome by introduction of thermo-cleavable tert-butoxycarbonyl (t-Boc) groups, to enhance solubility during thin film device processing.

Here, we present synthesized symmetrical dibromo, diphenyl, and dinaphthalenyl indigo derivatives (compounds denoted as **InBr**, **InPh**, and **InNap**). Direct halogenation of indigo has been used or the first time, during the synthesis of dihaloindigo. Latent pigment analogues of the studied compounds decorated by t-Boc groups were also synthesized. A post-deposition thermal treatment process is then utilized, to remove the protecting t-Boc groups and produce semiconductor thin films. The studied compounds (InBr, InPh, and InNap) show an optical band gap of 1.6-1.8 eV, while their t-Bocprotected forms have a band gap of approximately 2.1 eV. The compounds were studied in organic field-effect transistors (OFETs) to assess the field-effect mobility of charge carriers in the materials. In case of physical vapordeposited (PVD) films in AlO<sub>x</sub>/TTC dielectric OFETs, the compounds showed p-type charge transport with a hole mobility of up to 2.2×10<sup>-2</sup> cm<sup>2</sup>V<sup>-1</sup>s<sup>-1</sup> in. Moreover, dibromo derivative (InBr) showed ambipolar charge transport, featuring electron mobility of up to  $1.1 \times 10^{-3}$  cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup> in an electron transport enhancing setup. Contrary to the previously described usual experience [5], the compound InNap, retained the form of a homogenous film even after the thermal treatment deprotection.

#### References

- [1] E.D. Głowacki, G. Voss, L. Leonat, M. Irimia-Vladu, S. Bauer, N.S. Sariciftci, Isr. J. Chem. 52 (2012) 540–551.
- [2] M. Irimia-Vladu, E.D. Głowacki, P.A. Troshin, G. Schwabegger, L. Leonat, D.K. Susarova, O. Krystal, M. Ullah, Y. Kanbur, M.A. Bodea, V.F. Razumov, H. Sitter, S. Bauer, N.S. Sariciftci, *Adv. Mater.* 24 (2012) 375–380.

[3] M. Irimia-Vladu, P.A. Troshin, M. Reisinger, G. Schwabegger, M. Ullah, R. Schwoediauer, A. Mumyatov, M. Bodea, J.W. Fergus, V.F. Razumov, *Org. Electron*. 11 (2010) 1974–1990.

[4] M. Irimia-Vladu, P.A. Troshin, M. Reisinger, L. Shmygleva, Y. Kanbur, G. Schwabegger, M. Bodea, R. Schwödiauer, A. Mumyatov, J.W. Fergus, V.F. Razumov, H. Sitter, N.S. Sariciftci, S. Bauer, *Adv. Funct. Mater.* 20 (2010) 4069–4076.

[5] E.D. Głowacki, G. Voss, K. Demirak, M. Havlicek, N. Sünger, A.C. Okur, U. Monkowius, J. Gąsiorowski, L. Leonata, N.S. Sariciftci, *Chem. Commun.*, 2013,49, 6063-6065

#### Acknowledgement

Authors gratefully acknowledge funding from INTER-EXCELLENCE project LTAIN19006. Authors are thankful to the LIOS, JKU Linz for possibility to use the facilities. Authors acknowledge FCH, BUT and IISER Kolkata facilities.

# PO10: Novel Conductive PEDOT:DBSA Hydrogel Exhibits Tunable Properties for Bioelectronics

**Malečková Romana**<sup>1</sup>, Tumová Šárka<sup>1</sup>, Marková Aneta<sup>1</sup>, Pospíšil Jan<sup>1</sup>, Smilek Jiří<sup>1</sup>, Pešková Michaela<sup>2, 3</sup>, Kubáč Lubomír<sup>4</sup>, Víteček Jan<sup>2</sup>, Vala Martin<sup>1</sup>, Weiter Martin<sup>1</sup>

- <sup>1</sup> Faculty of Chemistry, Brno University of Technology, Purkyňova 464/118, 612 00 Brno, Czech Republic, Email: Romana.Maleckova@vut.cz
- <sup>2</sup> Department of Biophysics of Immune System, Institute of Biophysics of the Czech Academy of Sciences, Královopolská 135, 612 65 Brno, Czech Republic
- <sup>3</sup> Department of Biochemistry, Faculty of Science, Masaryk University, Kamenice 5, 625 00 Brno, Czech Republic
- <sup>4</sup> Centre for Organic Chemistry, Rybitví 296, 533 54 Rybitví, Czech Republic

Keywords: PEDOT, conductive hydrogels, impedance spectroscopy, mechanical properties

Bioelectronic devices can help us greatly with tissue stimulation, precise sensing of biological signals, or efficient drug delivery within the therapeutic window. Devices, which are routinely used nowadays, are usually based on conducting polymers in the form of thin films. However, thin films are physically and mechanically completely different from soft biological tissues. As opposed to thin films, tissues are 3-dimensional environments full of water, which makes them very soft. Especially when in long-term contact, these differences at the tissue-device interface inevitably result in material incompatibility with biological tissues and limited efficiency of the device [1].

Hydrogels are 3-dimensional networks rich in water content; in this way, their mechanical and physical properties mimic the properties of biological tissues. Pure conducting hydrogels have emerged only recently and, because of their high compatibility with tissues and mixed ionic-electronic conductivity, they seem to be very promising candidates for more efficient bioelectronics. However, the preparatory processes of such hydrogels often require the use of nonconductive hydrogel templates or complicated preparatory processes involving high temperatures. Furthermore, most existing conductive hydrogels are based on PEDOT:PSS, whose biocompatibility was shown to be insufficient for some applications [2].

In this work, we prepared a conductive hydrogel based on a novel polymer composite PEDOT:DBSA, for cell stimulation in regenerative medicine. The preparatory process is facile and does not involve the use of nonconductive hydrogel templates. The hydrogel possesses excellent biocompatibility towards murine endothelial cells. The mechanical properties are tunable and in the range of soft biological tissues. The hydrogel shows low impedance at 1 Hz and mixed ionic-electronic conductivity, where the electronic one is one order of magnitude higher than the conductivity of biological tissues. Thus, this material holds the promise to form a truly functional interface between tissues and the bioelectronic device.



Figure 1: Summary of preparation and properties of pure conductive hydrogel based on novel PEDOT:DBSA

#### References

- [1] Z. Hao, S. Wang, K. Zhang, J. Zhou, D. Li, J. He, L. Gao, L. Wang, *Materials* 14 (2021), 4718.
- [2] E. Šafaříková, L. Švihálková, S. Stříteský, L. Kubala, M. Vala, M. Weiter, J. Víteček, Sensors and Actuators B (2018) 418-425

#### Acknowledgement

This work was supported by the Czech Science Foundation, grants No. 21-01057S and No. 24-10469S. The authors would also like to acknowledge the support of Brno University of Technology, project CEITEC VUT/FCH-J-21-7268.

# PO11: Real-time Study of Ion Exchange and Transport in Organic Bioelectronic Devices

**Marková Aneta**<sup>1</sup>, Donghak Byun<sup>2</sup>, Ivaylo Zhivkov<sup>1</sup>, Jan Víteček<sup>3</sup>, Johannes Bintinger<sup>2</sup>, Martin Weiter<sup>1</sup>, Martin Vala<sup>1</sup>

- <sup>1</sup> Brno University of Technology, Faculty of Chemistry, Purkyňova 464/118, 612 00 Brno, Email: vala@fch.vut.cz
- <sup>2</sup> Linköping University, Laboratory of Organic Electronics, Bredgatan 33, 602 21 Norrköping, Sweden
- <sup>3</sup> Institute of Biophysics of the Czech Academy of Sciences, Department of Biophysics of Immune System, Královopolská 135, 612 65 Brno

Keywords: organic electrochemical transistor, OECT, organic electronic ion pump, OEIP, electrical detection, absorbance, ion exchange, ion transport

An increasing number of various civilization diseases such as Parkinson's and Alzheimer's diseases, epileptic seizures, heart attack, other heart diseases, depression, diabetes, and cancer, and the necessity to treat them calls for novel targeted treatments with maximum efficiency but minimum side effects. Such possibility of targeted dosing of drugs in space and time with electronic precision brings organic bioelectronics. Two very promising devices are organic electronic ion pumps (OEIP) and organic electrochemical transistors (OECT).

The OECT is based on ion exchange and ion transport in organic semiconductors and OEIP is based on ion transport through ion-selective membranes. Both devices have a unique ability to conduct ions in addition to electrons. The polymer structure with lower Young's modulus and mixed ionic-electronic conductivity makes these devices much more efficient at transferring information between living tissue and devices than today's devices.

This work focuses on the real-time study of ion exchange and transport in these two devices. Even though there was significant progress in research, the understanding of ion transport and ion exchange is derived mostly based on nonspecific or non-real-time detection methods. A precise understanding of the role of ions is critical for understanding the principle of operation of organic (bio)electronic devices.

In this work, we combine electrical, optical, and direct pH measurements to measure and evaluate the number of exchanged and transported ions directly. The outputs of all detection methods are correlated. The advantage of this method is that the amount of ions is determined directly in situ and in real-time. Based on this method we can study the transport properties of different drugs in membranes and organic semiconductors.



Figure 1: Schema of the combined detection of ion exchange in an organic electrochemical transistor

#### Acknowledgement

The work was supported by the Czech Science Foundation, project no. 24-10469S.

## PO12: Graphitic Carbon Nitride Coatings with Enhanced Porosity

#### Patakyová Sylvia<sup>1</sup>, Dzik Petr<sup>1</sup>, Veselý Michal<sup>2</sup>

<sup>1</sup> Brno University of Technology, Faculty of Chemistry, Purkyova 464/118, Brno, 612 00, Czech Republic, Email: Sylvia.Patakyova@vut.cz

#### Keywords: graphitic carbon nitride, coatings, porosity, photocatalytic activity

Since its discovery in 2006, graphitic carbon nitride (GCN) has attracted considerable interest due to its photocatalytic activity, despite being a well-known substance [1, 2]. GCN consists of tri-s-triazine rings crosslinked by trigonal N atoms <sup>[3]</sup>. Its key advantage is being a metal-free medium band gap semiconductor with high thermal and chemical stability, along with a customizable electronic structure. Due to its properties, the material is promising for various applications. The electronic bandgap of GCN is approximately 2.7 eV, which is lower than the 3.2 eV band gap of titanium dioxide (TiO<sub>2</sub>), the standard for photocatalytic materials [3]. Based on its electronic structure, GCN should be capable of releasing oxygen and hydrogen through water splitting. Additionally, GCN is easy and inexpensive to synthesize which makes it an attractive semiconductor for large-scale applications.

This report outlines the fabrication and properties of durable GCN coatings with enhanced porosity.

The patented oligomeric siloxane binder ensures the adhesion and cohesion of these coatings [4].

GCN was synthesized from a melamine-cyanurate complex. The crude GCN was subjected to wet ball milling in isobutanol to produce a suspension of GCN particles with a narrow size distribution, ideal for coating. After milling, a coating was prepared by incorporating a variable amount of siloxane binder and a pore-forming agent, camphor. Substrates (plain soda lime glass or FTO glass) were coated using a Mayer rod film applicator. Camphor was sublimed from the coated substrates by heating them to 80 °C under reduced pressure. This process left voids in the coatings. The shape of these voids was strongly influenced by the camphor concentration.

The mechanical, physical and chemical properties of the fabricated coatings were investigated in detail by various methods. The photocatalytic activity was evaluated with several model pollutants to determine the optimal pore-forming agent content. We have demonstrated that the porous texture improves photocatalytic activity by improving mass transfer and light penetration into the catalyst layer.

#### References

- [1] F. Goettmann et al., Angewandte Chemie-International Edition 45 (2006) 4467-4471.
- [2] F. Goettmann et al., *Chemical Communications* 43 (2006) 4530-4532.
- [3] X.C. Wang, S. Blechert, M. Antonietti, Acs Catalysis 2 (2012) 1596-1606.
- [4] T. Svoboda, M. Veselý, R. Bartoš, T. Homola, P. Dzik, *Catalysts* 11 (2021) 50.

#### Acknowledgment

This work received financial support from the Grant Agency of the Czech Republic through project 23-06843S.

# PO13: Diffusion Model for Halide Perovskites via Impedance Spectroscopy

Jan Pospisil<sup>1</sup>

<sup>1</sup> Faculty of Chemistry, Brno University of Technology, Purkyňova 118, Brno, 61200, Czech Republic, Email: pospisilj@fch.vut.cz

A universal approach to the calculation of diffusion coefficients in lead halide perovskite single crystals having ionic and mixed ionic-electronic conductivity is presented. Using impedance spectroscopy, it is demonstrated how to model a non-ideal Warburg element and the equivalent circuit of a transmission line to identify ion diffusion in a material. The proposed method is applicable to samples of any thickness and electrical properties. In addition, it is shown how to overcome the problems of measuring low-frequency impedance and non-ideal behavior of elements using extrapolative modeling and approximation.

# PO14: Flavin-Inspired Electrocatalysts Towards Sustainable Hydrogen Production

Richtár Jan<sup>1</sup>, Apaydin Dogukan H<sup>2</sup>, Ivanová Lucia<sup>1</sup>, Krajčovič Jozef<sup>1</sup>

- <sup>1</sup> Institute of Chemistry and Technology of Environmental Protection, FCH BUT, Purkyňova 464/118, Brno, Czech Republic, Email: jan.richtar@fch.vut.cz
- <sup>2</sup> Faculty of Technical Chemistry, TU Vienna, Getreidemarkt 9/165, Wien, Austria

Keywords: hydrogen production, electrocatalysis, bio-inspired materials, flavins

The global need for energy has significantly risen in recent decades and is supplied mostly by fossil fuels which account for around 80 % total energy demands. Therefore, renewable sources of energy have been pointed in the centre of interest. Among them, hydrogen economy can address the utmost need for a transition to the green energy. To date, however, vast majority of hydrogen is produced by steam-methane reforming. On the other hand, low-emission production comprised less than 1% in 2022. Low emission hydrogen production can be achieved by electrolysis of water with overall equation  $2H_2O \rightarrow 2H_2 + O_2$ , driven by renewable electricity sources. Being kinetically sluggish, the electrocatalytic HER is often mediated by catalysts.

Massive upscale of effective electrolytic water splitting should be promoted by materials with low socioecological footprint which can be addressed by sustainable and recyclable organic electrocatalysts. Increasingly, bioinspired organic materials emerge as robust and stable electrocatalysts with fine-tunable structure and properties (e.g. emeraldine-polyguanine or polydopamine, mimicking platinum surface).<sup>1</sup>

Flavins are ubiquitous cofactors of enzymatic redox reactions involving transfer of one or two electrons

occurring over wide potential range which translated also in numerous applications. Riboflavin and its electropolymerized form coated on a carbon electrode serve as excellent electron shuttles promoting electron uptake in microbial fuel cells. Moreover, polyriboflavin proved to be active in oxygen evolution reaction.<sup>2</sup> Redoxactive part of riboflavin can be minimized to pteridine-2,4dione moiety important for preserving the diazabutadiene moiety. On the other hand, expansion of the conjugated system is desirable for tuning of the optical and electrochemical properties.<sup>3</sup>

We present a versatile synthetic approach towards advanced non-fused NH-free flavin derivatives and their initial evaluation as electrocatalysts for hydrogen evolution. Both small-molecular and polymer materials were synthesized and investigated via electrochemical measurements followed by electrolytic experiments. Electrocatalytic activity of some metal-free flavin materials was observed in terms of several fold increase in amount of evolved hydrogen. Versatility of the synthesis of flavinbased small molecules and corresponding polymers enables enlarging of the portfolio of the catalysts for deeper experiments and potential applications in HER.



Figure 1: Synthetic approach to target flavin materials

#### References

- [1] Coskun, H., et al.. Adv. Mater. Interfaces 7 (2020) 1901364.
- [2] Kleinbruckner, N., et al. Adv. Sustainable Syst. (2023) 2300352-2300360.
- [3] Richtár, J., et. al. *Molecules* 23 (2018) 2271.

#### Acknowledgement

Research has been supported by Aktion projects 95p3 and 98p15.

## PO15: Bio-inspired Polymers for CO<sub>2</sub> Capture and O<sub>2</sub> Reduction

**Schimanofsky Corina**<sup>1</sup>, Kleinbruckner Nadine<sup>1</sup>, Leeb Elisabeth<sup>1</sup>, Wielend Dominik<sup>1</sup>, Irimia-Vladu Mihai<sup>1</sup>, Sariciftci Niyazi Serdar<sup>1</sup>

<sup>1</sup> Linz Institute for Organic Solar Cells (LIOS) / Institute of Physical Chemistry, Johannes Kepler University Linz, Altenberger Straße 69, 4040 Linz, Austria, Email: corina.schimanofsky@jku.at

#### Keywords: Antraquinone, Riboflavin, Polymers, CO<sub>2</sub> Capture, O<sub>2</sub> Reduction

There are currently increased research efforts to make industrial processes more climate-friendly and reducing their dependence on fossil fuels. To achieve this goal, biomaterials are gaining more and more attention, even if they are not yet completely climate-neutral [1]. Promising naturally occurring organic molecules for this are the classes of anthraquinone and riboflavin (Vitamin B2). Both the monomers and the polymers of these two classes are known to have good electrocatalytic properties for carbon dioxide ( $CO_2$ ) capture and oxygen ( $O_2$ ) reduction toward hydrogen peroxide ( $H_2O_2$ ) [2-5]. Furthermore, the monomers and polymers can in addition be used in organic batteries, sensors, and as electrodes in various devices [6,7].

In this approach, we worked on the successful electropolymerization and immobilization of the

1-aminoanthraquinone and riboflavin on different carbon-based electrodes as well as on an optically transparent electrode, which gives rise to further application in optoelectronic devices. The resulting polymers were characterized using infrared spectroscopy and scanning electron microscopy (SEM) to gain insights into the structure-property relationships. These two techniques also provide a suitable proof of the successful polymerization of these biomaterials. Cyclic voltammetry (CV) of these polymers was performed to provide information about the redox properties and the stability of the resulting polymers. Furthermore, CVs were performed to prove the capability of electrochemical CO<sub>2</sub> capture and O<sub>2</sub> reduction of the materials [8].

#### References

- [1] E.A.R. Zuiderveen, K.J.J. Kuipers, C. Cladeira, S.V. Hanssen, M.K. van der Hulst, M.M.J. de Jonge, A. Vlysidis, R. van Zelm, S. Sala, M.A.J. Huijbregets, *Nature Communications* 14 (2023) 8521.
- [2] A. Kormanyos, M.S. Hossain, G. Ghadimkhani, J.J. Johnson, C. Janaky, N.R. de Tacconi, F.W. Foss Jr., Y. Paz, K. Rajehwar, *Chemistry-A European Journal* 22 (2016) 9209-9217.
- [3] C. Schimanofsky, D. Wielend, S. Kröll, S. Lerch, D. Werner, J.M. Gallmetzer, F. Mayr, H. Neugebauer, M. Irimia-Vladu, E. Portenkirchenr, T. S. Hofer, N.S. Sariciftci, *J. Phys. Chem* 126 (2022), 14138-14154.
- [4] A. Kerschbaumer, D. Wielend, E. Leeb, C. Schimanofsky, N. Kleinbruckner, H. Neugebauer, M. Irimia-Vladu, N.S. Sariciftci, *Catal Sci Technol* 13 (2022) 834-843.
- [5] E. Leeb, D. Wielend, C. Schimanofsky, N.S. Sariciftci, *Electrochem. Sci. Adv.* 2 (2022) e202100211.
- [6] M.R. Gerhardt, L. Tong, R. Gomez-Bombarelli, Q. Chen, M.P. Marshak, C.J.Galvin, A. Aspuru-Guzik, R. G. Gordon, M.J. Aziz, *Adv. Energy Mater.* 7 (2017) 1601488.
- [7] W. A. Badawy, K.M. Ismail, S.S. Medany, Zeitschrift für Physikalische Chemie 227 (2013) 1741-1757.
- [8] N. Kleinbruckner, E. Leeb, D. Wielend, C. Schimanofsky, M. Cobet, F. Mayr, A. Kerschbaumer, C. Yumusak, J. Richtar,
- M.C. Scharber, H. Neugebauer, M. Irimia. Vladu, J. Krajcovic, N.S. Sariciftci, Sustainable Syst. 8 (2024) 2300352.

#### Acknowledgement

The author wants to thank all the co-workers for their help. Furthermore, all the authors thank the financial support of the Austrian Agency for International Cooperation in Education and Research (OeAD-GmBH, WTZ, CZ01/2020, 8J20AT025). In addition, we gratefully acknowledge financial support from the Austrian Science Foundation (FWF) within the Wittgenstein Prize from Prof. Sariciftci (Z222-N19), and from the European Research Executive Agency within the Project EINSTEIN (Project No. 101136377, HORIZEN-WIDERE-2023-ACCESS-03).

# PO16: Enhanced Fluorescence in Stilbene-Based Photoluminescent Materials: Host-Guest Systems and Förster Resonance Energy Transfer for Far-Red and White-Light Emission

**Smolka Rastislav**<sup>1</sup>, Kolaříková Adéla<sup>1</sup>, Čekal Jozef<sup>1</sup>, Pauk Karel<sup>2</sup>, Luňák Stanislav Jr.<sup>1</sup>, Imramovský Aleš<sup>2</sup>, Vala Martin<sup>1</sup>

- <sup>1</sup> Materials Research Centre, Faculty of Chemistry, Brno University of Technology, Purkyňova 464/118, CZ-612 00 Brno, Czech Republic, Email: Rastislav.Smolka@vut.cz
- <sup>2</sup> Institute of Organic chemistry and Technology, Faculty of Chemical Technology, University of Pardubice, Studentská 95, CZ-530 09 Pardubice, Czech Republic

Keywords: Photoluminescence, Host-guest (HG) systems, Förster resonance energy transfer (FRET), White-light emitting (WLE) materials, Far-red (FR) fluorescence

Organic conjugated molecules have garnered significant attention over the past decades due to their unique optical properties, tuneable colours, and versatile applications [1]. In this study emphasis will be placed on the characterization of stilbene-based photoluminescence materials and their properties in solid-state and molecular mixtures. Fluorescence properties of studied materials primarily come from an intramolecular electronic transition of charge-transfer (CT) character. With this approach it is possible to design materials with wide range of colour emission [2].

In case of red-emitting materials, such approach leads to narrowing the band-gap and reduction of solid-state fluorescence quantum yields due to the promotion of intramolecular non-radiative processes. To improve fluorescence in far-red (FR) part of spectrum so-called host-guest systems (HG) can be utilized [3]. HG systems are binary mixtures of structurally similar molecules with different band gab energies resulting in different colour of emitted light. In such systems the effect of Förster resonance energy transfer (FRET) between two components of a mixture, where one acts as donor of energy and other as acceptor of energy, increases the fluorescence quantum yield of an acceptor fluorophore beyond its usual level. Such systems are deployed in the form of nanoparticles, showing increased intensity of acceptor-like photoluminescence.

If the donor-acceptor pair of molecules and their ratio is carefully selected it is possible to achieve only partial energy transfer leading to creation of systems in which the emission of both components persists. With this approach it is possible to obtain bright with-light emitting (WLE) materials.

Intense solid-state fluorescence materials are highly desirable for various applications. WLE materials are used in light-emitting field-effect transistors or organic lightemitting diodes (OLEDs) where the basis consists of whitelight emitting layer [4]. FR emitting materials are especially important in form of water-dispersible nanoparticles for bioimaging. By utilizing these materials, fluorescence imaging benefits from decreased self-fluorescence in the FR region; the impact of light scattering is reduced, thus the far-red fluorescence is much less affected. Moreover, red light demonstrates higher penetrability in biological tissue. This allows for higher optical contrast and reduced photodamage [5].

#### References

- [1] M. Shimizu, T. Hiyama, *Chemistry An Asian Journal* 5 (2010) 1516-1531.
- [2] K. Pauk, S. Luňák, A. Růžička, et al., RSC Advances 12 (2022) 34797-34807.
- [3] H. Yao, K. Ashiba, ChemPhysChem 13 (2012) 2703-2710.
- [4] Z. Chen, C. L. Ho, L. Wang, W. Y. Wong, Advanced Materials 32 (2020).
- [5] J. Wu, Z. Shi, L. Zhu, et al., Advanced Optical Materials 10 (2022).

# PO17: Investigating the Spectroscopy of Lumazine and Flavin in the DMSO-Water Mixture

**Jan Truksa**<sup>1</sup>, Matouš Kratochvíl<sup>1</sup>, Jan Richtár<sup>1</sup>, Lucia Ivanová<sup>1</sup>, Martin Weiter<sup>1</sup>, Jozef Krajčovič<sup>1</sup>, Vladimír Lukeš<sup>3</sup>

- <sup>1</sup> Faculty of Chemistry, Brno University of Technology, Purkyňova 118, CZ-612 00 Brno, Czech Republic, Email: Jan.Truksa@fch.vut.cz
- <sup>2</sup> Institute of Physical Chemistry and Chemical Physics, Slovak University of Technology in Bratislava, Radlinského 9, SK-812 37 Bratislava, Slovakia

Keywords: Alloxazine, Flavins, Vertical excited states, Fluorescence, Dyes, Tautomerisation

The absorption and emission spectra were investigated for four molecules – lumazine and its cyanated derivative (Fig. 1. a) on the left) and alloxazine and its fluorinated derivative (Fig. 1. a) on the right), with dimethyl sulfoxide (DMSO) serving as the primary solvent. To modulate the spectroscopic properties, water was progressively added to the DMSO. Interesting effects were found, especially in the case of the cyanated derivative, where the addition of water results in a uniform blue shift, shown in Fig. 1. b).

Further intriguing results were found for the samples containing 65 % of water and 35 % of DMSO. In this case, a notable decrease in absorption and emission intensities was registered, even larger than the water quenching observed in other cases. This is likely related to the

formation of DMSO·2H2O trimers that has been documented in this case [1]. A similar behavior has been found for acetonitrile mixtures in the past, and a possible use for probing microenvironments of solvent immediately surrounding an analyte has been suggested [2].

Finally, water solubility is greatly enhanced by the substitution of polar groups, making it easier to penetrate cell membranes than the larger flavins, which have been used for fluorescence imaging of living cells [3]. Therefore, these molecules could find broader use for example in in vitro imaging.

The spectroscopic properties of studied molecules were calculated using the density functional theory in the implicit DMSO solvent model and with explicit water molecules.



Fig. 1. a) the structures of the studied molecules; b) the effect of varying DMSO concentration on the absorption spectra.

#### References

- [1] I. Płowaś, J. Świergiel, J. Jadżyn, JCED 58(6), 1741-1746 (2013).
- [2] S. Dutta Choudhury, H. Pal, JPC B 120(46), 11970-11977 (2016)
- [3] A. Golczak, M. Insińska-Rak, A. Davoudpour, et al. SAA 272, (2022).

#### Acknowledgement

The work has been supported by Slovak Research and Development Agency (APVV-15-0053) and VEGA 1/0504/20. V.L. thanks to Ministry of Education, Science, Research and Sport of the Slovak Republic for funding within the scheme "Excellent research teams". We are grateful to the HPC center at the Slovak University of Technology in Bratislava, which is a part of the Slovak Infrastructure of High Performance Computing (SIVVP project, ITMS code 26230120002, funded by the European region development funds, ERDF) for the computational time and resources made available. The authors thank for financial support of this investigation by the Czech Science Foundation (project No. 21-01057S). J.K. thanks the project CZ.02.2.69/0.0/0.0/18\_053/0016962 of the Ministry of Education Youth and Sports of the Czech Republic. J.T., M.K. and L.I. thank to the internal grant FCH-S-22-8012 of the Brno University of Technology. Computational resources were supplied by the project "e-Infrastruktura CZ" (e-INFRA CZ LM2018140) supported by the Ministry of Education, Youth and Sports of the Czech Republic. L.I. Thanks the Brno City Municipality (Brno Ph.D. Talent Scholarship) for the financial support.

# PO18: Combined Detection Method as a New Approach for the Selective Study of Ion Exchange and Transport in Organic Bioelectronic Devices

Aneta Marková<sup>1</sup>, Donghak Byun<sup>2</sup>, Ivaylo Zhivkov<sup>1</sup>, Jan Víteček<sup>3</sup>, Johannes Bintinger<sup>2</sup>, Martin Weiter<sup>1</sup>, Vala Martin<sup>1</sup>

- <sup>1</sup> Brno University of Technology, Faculty of Chemistry, Purkyňova 464/118, 612 00 Brno, Email: vala@fch.vut.cz
- <sup>2</sup> Linköping University, Laboratory of Organic Electronics, Bredgatan 33, 602 21 Norrköping, Sweden
- <sup>3</sup> Institute of Biophysics of the Czech Academy of Sciences, Department of Biophysics of Immune System, Královopolská 135, 612 65 Brno

Keywords: organic electrochemical transistor, OECT, organic electronic ion pump, OEIP, electrical detection, stimulation, absorbance, ion exchange, ion transport, cell membrane

Organic bioelectronics is widely studied for a use as a target therapy for wide range of civilisation diseases such as Parkinson's disease, epileptic seizures, regeneration of damaged nerve connections, heart failure and diseases, depression, diabetes, or cancer. These devices offer high spatiotemporal control and thus potentially limiting, if not completely avoiding, side effects, which are common in conventional systemic treatments.

Very promising organic bioelectronic devices are the organic electronic ion pump (OEIP) and organic electrochemical transistor (OECT). Both are based on ion exchange and/or ion transport in organic semiconductors and ion-selective membranes. This ability to conduct ions in addition to electrons makes these devices very effective in signal transmission between living tissue and the device.

Although OEIP and OECT already proved to be suitable for many medical applications, the understanding of ion

transport and ion exchange is derived mostly based on nonspecific and/or nonreal-time detection methods. However, a precise understanding of the role of ions is critical for understanding the principle of operation of organic (bio)electronic devices.

To study the ion exchange and ion transport in OECT and OEIP we combined three independent detection methods, which detect ions continuously in situ. We use optical detection and chronoamperometry and in a case of protons we also use pH measurement. Based on the outputs of these methods, the amount of transferred/exchanged ions is calculated and correlated. This approach has the potential to be used to study the transport of ions and new drugs in pharmaceutical research when optimised.



Figure 1: Schema of the combined detection of ion transport in organic electronic ion pump

#### Acknowledgement

The work was supported by the Czech Science Foundation, project no. 24-10469S.

# PO19: Optical Properties Manipulation with Novel Phenylene-Thienyl Chalcone Derivatives

#### Veselý Dominik<sup>1</sup>, Georgiev Anton<sup>2</sup>, Krajčovič Jozef<sup>1</sup>

- <sup>1</sup> Faculty of Chemistry, Institute of Chemistry and Technology of Environmental Protection, Purkyňova 464/118, 612 00 Brno, Czech Republic, Email: Dominik.Vesely@vut.cz
- <sup>2</sup> Department of Organic Chemistry, University of Chemical Technology and Metallurgy, 8 St. Kliment Ohridski blvd, 1756 Sofia, Bulgaria

#### Keywords: Photochromism, Chalcones, Fluorescence switching, Aggregation-induced emission

Organic  $\pi$ -conjugated molecules play a fundamental role in the development of new functional materials with multi-stimuli response and applications. The manipulation of matter by changing the environment to influence the electronic distribution is a key factor in the design of new optical materials [1].

This work focuses on design, preparation and optical characterization of the phenylene-thienyl chalcone derivatives with various terminal groups – amino (**3a**), hydroxyl (**3b**) and carboxyl (**3c**). We were able to selectively manipulate the optical behavior via these functional groups simply by treatment under acidic or basic conditions. The photoluminescence quantum yield (PLQY) of the protonated ammonium salt was boosted to 10 % in comparison with 2 % in the neutral form. On the

other hand, deprotonation of the alkoxy and carboxy group led to the formation of a non-emissive anions due to the photoinduced electron transfer process. Moreover, we studied the behavior in the aqueous environment that resulted in the aggregation induced emission effect with a bathochromic shift and improved PLQY for all three chalcone compounds. Finally, only the compound **3c** showed a fluorescence in the solid-state with a broad emission band at 576 nm with a relatively high PLQY (18.6 %) [2].

With these results, we proved the potential for sensing applications of the prepared compounds as we could monitor the emission enhancement or quenching strongly depending on the environment.



Figure 1: Graphical demonstration of the optical properties study [2]

#### References

- [1] H.Q. Peng, et al., J. Am. Chem. Soc. 139 (2017) 29.
- [2] D. Vesely, et al., J. Mol. Liq. 397 (2024) 124119.

#### Acknowledgement

DV and JK thank the project No. FCH-S-24-8592 of Ministry of Education, Youth and Sports of the Czech Republic. AG thanks the project No. BG-RRP-2.004-0002, "BiOrgaMCT", Laboratory of Organic Functional Materials of Bulgaria.

Pushing innovation to create intelligent power and sensing technologies that solve the most challenging customer problems.

# onsemi









- ANAMET s.r.o.: Trusted supplier of laboratory and analytical equipment with over 25 years of experience on the Czech market.
- World-Class Products: Portfolio includes renowned brands like
  Elementar, Malvern Panalytical, 3P Instruments, Dataphysics, and Thermo Scientific.
- Elemental Analysis: Advanced tools from Elementar for analyzing non-metallic elements in organic and inorganic substances.
- Microscopy Solutions: Phenom electron microscopes from
  Thermo Scientific and atomic force microscopes from Nanosurf for in-depth sample analysis.
- Particle Size Determination: Cutting-edge instruments like
  MasterSizer, ZetaSizer, LUMiSizer, and LUMiReader for accurate particle size and suspension analysis.
- **Comprehensive Support:** Complete solutions for analytical chemistry, including expert consulting and service support.





www.anamet.cz

sales@anamet.cz





# **Discover world of Anton Paar**

12.-13. 9.2024

Together We Measure the World

9th Meeting on Chemistry & Life

Laboratory instruments, process sensors, measuring technology, automation

Highly accurate determination of physical quantities - density, viscosity, specific surface area, ...

Choose the perfect solution for your research and production

Local product support and service team

# GDP KORAL COMPOSITES



# **GDP KORAL**

is a leading technology company that designs, manufactures and markets composite profiles as well as complete parts for innovative applications in transportation and construction.

## Contact:

GDP KORAL s.r.o. Za Mlýnem 5, 666 01 Tišnov, Czech Republic www.gdpkoral.com marketing@gdpkoral.com

Holder of certificates ISO 9001 and 14001.

# HARTMANN

# Do you want to become part of our team?

At HARTMANN, we are driven by our desire to improve health care, desire that is based on more than 200 years of experience and that works in nearly 100 countries around the world.

Join us and take the opportunity to do work that matters.



hartmann.cz
#### Merck

# BIG SCIENCE SMALL FOOTPRINT

Sustainable lab products, solutions & services for responsible science

Ensuring a sustainable future together

Our mission is to ensure a more sustainable future for everyone. With our growing portfolio of greener products, programs and services, we now offer even more ways for you to practice responsible science.

Our solutions combine enhanced sustainability with exceptional quality, so they are better for the planet, and for your work.

**Your Opportunities** 

- Sustainable & less harmful alternatives
- Biodegradable & greener chemicals
- Waste reduction & sustainable packaging



Much more on SigmaAldrich.com/Sustainable-Chemistry

The life science business of Merck operates as MilliporeSigma in the U.S. and Canada.

© 2024 Merck KGaA, Darmstadt, Germany and/or its affiliates. All Rights Reserved. Merck, Millipore, Sigma-Aldrich, and Supelco are trademarks of Merck KGaA, Darmstadt, Germany or its affiliates. All other trademarks are the property of their respective owners. Detailed information on trademarks is available via publicly accessible resources. Sigma-Aldrich.

Lab & Production Materials

Supelco® Analytical Products

**Millipore**®

Preparation, Separation, Filtration & Monitoring Products





...you can measure both solid and liquid samples seamlessly, without waiting times or any need for system adjustments.

www.metrohm.cz

office@metrohm.cz

"Spot the detail, see the whole. Vidět detail, poznávat celek."





## Surface analysis and imaging

- Atomic force microscopy (AFM, bioAFM, UHV AFM)
- Nanoindentation and Tribology
- Surface analysis (XPS, SIMS, etc.)
- Tabletop Scanning Electron Microscopes (SEM)
- 3D optical and mechanical profilometers
- Electron microscope analyzers (EDS, WDS, EBSD, mXRF...)



# Thermal and mechanical analysis

- Thermogravimetric Analyzers
- Differential scanning Calorimeters
- Rheometers
- Dynamic mechanical testing
- Microcalorimetry
- Tensile and other mechanical testers



## X-Ray analytical techniques

- X-ray fluorescence spectrometers
- X-ray single crystal diffractometers
- X-ray fluorescence µ-XRF and TXRF
- X-ray powder diffractometers
- 3D X-Ray Microscopy (mCT, nCT)



#### Laboratory equipment

- Glove boxes, GMS, Purification systems
- Nanoindentation and AFM Probes and another accessories
- XRF consumables
- Mills, presses and sieves
- Fusion machines
- Presses



#### Měřicí technika Morava, s.r.o.

www.mt-m.eu





World leader in materials and component testing and your partner for accurate, reliable, reproducible and traceable results. A fundamental prerequisite for obtaining these test results is the perfect interplay of all components within the entire system which we design and produce all by our ourselves.

- / Universal testing machine for tensile and compression
- / Dynamic and fatigue testing systems
- / Creep testing machines
- / Load cells, specimen grips and extensometers
- / Temperature and environmental chambers
- / Pendulum impact testers
- / Drop weight testers
- / Hardness testers
- / Extrusion plastometers
- / HDT/Vicat
- / Automated testing solutions
- / Specimen preparation

#### ... you don't have to test anything else

ZwickRoell s.r.o. • Podnikatelská 2956/6 • 612 00 Brno



