



NANOAPP 2024

Nanomaterials & Applications

18 - 24 June 2024, Ptuj, Slovenia

BOOK OF ABSTRACTS

5th International Scientific Conference

NANOAPP 2024 - Nanomaterials & Applications



Ptuj, 18 - 24 June, 2024, Slovenia

Book of Abstracts | Zbornik povzetkov

**NANOAPP International Scientific Conference on Nanomaterials & Applications |
NANOAPP Mednarodna znanstvena konferenca Nanomateriali & aplikacije**

**5th International Scientific Conference NANOAPP 2024 – Nanomaterials & Applications |
5. Mednarodna znanstvena konferenca NANOAPP 2024 – Nanomateriali & aplikacije**

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NANOAPP International Scientific Conference on Nanomaterials & Applications |
NANOAPP Mednarodna znanstvena konferenca Nanomateriali & aplikacije

Venue | Prizorišče

Dominican Monastery, Ptuj, Slovenia | Minoritski samostan, Ptuj, Slovenija

Dates | Datum

18 – 24 June 2024 | 18. – 24. junij 2024

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FOREWORD

Welcome to the NANOAPP 2024 - Nanomaterials & Applications Conference in Ptuj, Slovenia

We are delighted to have you participate at the *NANOAPP 2024 - Nanomaterials & Applications Conference* (<http://nanoapp.ios.si/>) in **Dominican Monastery, Ptuj, Slovenia**, from **June 18th to 24th, 2024**.

It is **5th International Scientific Conference NANOAPP 2024 - Nanomaterials & Applications**, under the auspices of the **IOS, Institute for Environmental protection and Sensors d.o.o. & University of Maribor, the Faculty of Mechanical Engineering**.

The Scientific Committee consists of 7 top experts from 5 countries of the world. The meeting will consist of both oral and poster contributions.

At the *NANOAPP 2024 - Nanomaterials & Applications* meeting, world-renowned scientists in the field of *Hybrid Nanomaterials, Magnetic Nanomaterials, Nanomaterials & Photonics, Nanomaterials in Sensors, Sustainability and circular economy and Recycling - our future* will be present.

Great emphasis will also be placed on delivering information about the impact of nanomaterials and nanotechnology on the environment and human health.

We offer special thanks to the Co-chairs (from **Institute Charles Gerhardt Montpellier (ICGM)**, France; **ENS Lyon, University of Lyon, CNRS**, France; **Western Sydney University**, Australia), Organizing Committee, and The International Scientific Committee. We truly thank for the support of the sponsors and **exhibitor** companies (**Omega d.o.o.**, Slovenia) and the many on-site assistants for their tireless efforts in producing this event.

We hope you enjoy your stay in Ptuj and that you experience a truly valuable and memorable meeting.

Chair
of the NANOAPP 2024 - Nanomaterials &
Applications Conference

Prof. Dr. Aleksandra Lobnik




PROGRAMME
Day 1: Tuesday, 18th June 2024

	Registration - Dominican Monastery, Ptuj, Slovenia
Session 1	Recycling - our future
Session Chair	Prof. Dr. Aleksandra Lobnik, IOS, UMFS, Slovenia
14:00 – 15:15	Round Table: Recycling – our future Dr. Määttänen Marjo – VTT, Finland, PESCO project Coordinator Dr. Bojan Pahor, Project Manager, Saubermacher Slovenia Dr. Mojca Poberžnik, Head of the Environmental Protection/Recycling processes, IOS, Slovenia MSc. Lutz Walter, The European Technology Platform for the Future of Textiles and Clothing Denis Jahić; General Manager and Board Member, AquafilSLO MSc. Patricia Urban, CEPS (The Centre for European Policy Studies): Policies for textiles circularity
Session 2	Sustainability and circular economy
Session Chair	Määttänen Marjo, VTT, Finland
15:15 - 15:35	IL1: MSc. Satu-Marja Mäkelä, VTT, Finland - AI and data throughout circular textile flow
15:35 - 15:55	IL2: MSc. Alen Erjavec, UM FS, Slovenia - Enhancing Personal Protective Equipment Waste Recycling: A Comprehensive Analysis of Polymer Recyclates from Disposable Surgical Masks
15:55 - 16:30	Coffee Break
16:30 - 16:50	IL3: Dr. Mojca Poberžnik, IOS, Slovenia - Towards secondary raw materials
16:50 - 17:10	IL4: Ramon Pragt, T4E&CuRe, Netherlands - Low energy textile recycling
17:10 - 17:30	IL5: Dr. Heli Kangas, Valmet, Finland - Piloting and scaling-up textile recycling – challenges, solutions and opportunities
19:00 - 21:00	NANOAPP 2024 Conference Welcome Party


Day 2: Wednesday, 19th June 2024

Session 3	NANOAPP 2024 Opening Remarks
9:15 - 9:30	Prof. Dr. Aleksandra Lobnik, UM FS, IOS Prof. Dr. Lidija Fras Zemljič, Vice Dean, UM FS
Session 4	Nanomaterials & Hybrid Nanomaterials
Session Chair	Prof. Dr. John Bartlett, Australia
9:30 - 10:15	PL1: Prof. Dr. Corine Gerardin, France - Controlling interactions at interfaces to determine the molecular and nanometric structures of functional mesoporous materials
10:15 - 10:45	KL1: Prof. Dr. V. G. Kessler, Sweden - Polyoxometalate species as models of sol-gel metal oxide nanoparticles
10:45 – 11:15	Coffee Break
Session Chair	Prof. Dr. Galo Juan De Avila Arturo Soler Illia, Argentina
11:15 - 11:45	KL2: Prof. Dr. John Bartlett, Australia - Modulating textural and chemical properties in mesoporous organosilicas – the effect of addition sequence
11:45 - 12:15	KL3: Prof. Dr. Nicola Hüsing, Austria - Silicon polyolates: Opportunities and challenges in materials synthesis
12:15 - 12:45	KL4: Prof. Dr. Masahide Takahashi, Japan - Infrared crystallography for evaluation of framework and linker orientation in metal-organic framework films
12:45 - 13:15	KL5: Prof. Dr. Benoît Heinrichs, Belgium - Optimization of a synthesis procedure of nanocomposites silica/aliphatic polyesters by reactive extrusion for medical applications
13:15 – 15:00	Lunch
Session 5	Sustainability and circular economy
Session Chair	Prof. Dr. Beatriz Julián-López, Spain
15:00 - 15:30	KL6: Prof. Dr. Urban Bren, Slovenia - Molecular Mechanism of Antimicrobial Activity of Tannins Through Joint Experimental and Computational Techniques
15:30 - 15:50	IL6: Dr. Žiga Zebec, Slovenia - Production of terpenes from textile waste
Session 6	Nanomaterials & Sensors
Session Chair	Prof. Dr. Stephane Parola, France
15:50 - 16:20	KL7: Prof. Dr. Ivana Murković Steinberg, Croatia - Towards wearable (bio)chemical sensing with biocompatible functional nanomaterials
16:20 - 16:40	IL7: Dr. Inna Melnyk, Slovakia - The role of lanthanides and dyes in enhancing the photoluminescence of silica sensors for pharmaceutical monitoring in water
16:40 - 17:00	OL1: MSc. Allwin Mabes Raj - Advancing Mercury Detection: A MerB (Organomercurial-lyase)-based Solid-State Voltammetry Sensor for Methylmercury detection
17:00 - 18:00	Poster Session
18:30 - 21:00	Guided city tour and wine tasting


Day 3: Thursday, 20th June 2024

Session 7	Nanomaterials & Hybrid Nanomaterials
Session Chair	Prof. Dr. Corine Gerardin, France
9:30 – 10:15	PL2: Prof. Dr. Galo Soler Illia, Argentina - Programmable Nanosystems Through Chemical Pathways
10:15 - 10:45	KL8: Prof. Dr. Beatriz Julián-López, Spain - Advancing Scalability and Sustainability of Perovskite Nanocrystals Manufacturing for Photovoltaic and Optoelectronic Applications
10:45 - 11:15	KL9: Prof. Dr. Gulaim Seisenbaeva, Sweden - Design and synthetic approaches to hybrid adsorbents and bio-catalysts
11:15 - 12:00	Coffee Break
Session 8	Magnetic Nanomaterials & Applications
Session Chair	Prof. Dr. V. G. Kessler, Sweden
12:00 - 12:30	KL10: Prof. Dr. Spomenka Kobe, Slovenia - Sustainable Processing of Innovative Rare-Earth Magnets
12:30 - 12:50	IL8: Prof. Dr. Darja Lisjak, Slovenia - Electrical sensitization of magnetic nanoplatelets
12:50 - 13:10	IL9: Prof. Dr. Darko Makovec, Slovenia - Ceria-Based Nanocomposites for Catalysis by Magnetic Heating
13:10 - 14:30	Lunch
Session 9	Sustainability and circular economy
Session Chair	Prof. Dr. Masahide Takahashi, Japan
14:30 - 14:50	IL10: Prof. Dr. Matej Zdravec, Slovenia - Implementing a supportive environment for lifelong learning for sustainable engineering (Green2Eng)
14:50 - 15:10	OL2: MSc. Edoardo Donà - Plasma-Modification of graphene oxide for advanced ammonia
Session Chair	Prof. Dr. Sidney Jose Lima Ribeiro, Brazil
15:10 - 15:40	KL11: Dr. David Ravnjak, Slovenia - A novel approach in the use of bacterial nanocellulose for production of packaging films
15:40 - 16:10	KL12: Dr. Matej Bračič, Slovenia - Nanocoatings from Biopolymers
16:10 - 16:40	KL13: Prof. Dr. Vanja Kokol, Slovenia - Cellulose nanomaterials in innovative and emerging applications for sustainable and recyclable economy
16:40 - 17:00	OL3: MSc. Özkan Yapar - Advanced regenerated cellulose materials for emerging applications
17:00 - 18:00	Poster Session
19:00 - 22:00	Conference Dinner at Dominican Monastery



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Day 4: Friday, 21st June 2024

Session 10	Nanomaterials & Photonics
Session Chair	Prof. Dr. Nicola Hüsing, Austria
9:30 – 10:15	PL3: Prof. Dr. Sidney Jose Lima Ribeiro, Brazil - Photonic applications of Organic-Inorganic Hybrids. From direction modulated photoluminescence to cellulose aerogels for environmental applications
10:15 - 10:45	KL14: Prof. Dr. Stephane Parola, France - Playing with the plasmonic properties of metal nanoparticles : single particles, colloidal self-assemblies and hybrid plasmonic glasses
10:45 - 11:15	KL15: Prof. Dr. Uroš Cvelbar, Slovenia - Plasma nanofabrication for advanced SERS detection
11:15 - 11:45	KL16: Prof. Dr. Mladen Franko, Slovenia - Characterisation of Thin Films and Nanolayered Composite Materials by Photothermal Techniques
11:45 - 12:05	OL4: Prof. Dr. Aleksandra Lobnik, Slovenia - OpenLOOP Recycling project presentation
12:05 - 13:00	Farewell Party



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PLENARY LECTURES



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Controlling interactions at interfaces to determine the molecular and nanometric structures of functional mesoporous materials

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Ordered mesoporous silica resulting from the synergy between supramolecular self-assembly of macromolecular compounds and sol-gel processes present unique porous textural and surface properties, which make them attractive as drug delivery systems, sensors, adsorbents, catalysts, ion conductors and more generally for various applications in the fields of health, environment and energy. The control of their structure at the nanoscale is mainly governed by the form factor of the amphiphilic entities and their interactions with the inorganic precursors under specific physicochemical conditions of the synthesis. Different types of interactions (hydrogen bonding, van der Waals, electrostatic complexation) occur simultaneously and their cooperativity or competitiveness determine the structural parameters of the obtained materials : system curvature at the nanoscale, pore size, nature of the mesophase and wall thickness.

The functionalization of their mesopores is also a key step in their preparation for applications. Functionalization by organic, organometallic or bioactive groups can be achieved by well-controlled routes. But the introduction of polymers in the mesopores remains a major challenge. Yet, this could confer new properties to the materials. Conventional routes for polymer post-functionalization of mesopores do not allow to obtain dense and homogeneous distributions of polymers at the nanoscale. The use of polyion complex micelles (PICs) as structuring agents can overcome the problems encountered. PIC micelles are dynamic assemblies obtained by electrostatic complexation between a double-hydrophilic block copolymer and a polyelectrolyte auxiliary of micellization. Their formation is reversible in water as a function of pH and ionic strength. Their use is of major interest since they allow (1) the simple control of pore size and structure, (2) the recovery and recycling of pore-forming polymers, and (3) the direct preparation of structures functionalized by homogeneously distributed polymers. Another great advantage of the use of PIC micelles is the easy preparation of mesoporous nanoparticles of controlled size and morphology. Finally, the study of their formation mechanisms showed that the nature of the two polymer blocks and their preferential interactions with silica, with the micellization auxiliary or the solvent proved to be key parameters in controlling not only the internal porous interface of the material, but also its external surface and the material dimensionality.

References

1. J. Richard, *Chem. Mater.* (2022) 17, 7828. 2. J. Richard, *Micr. Meso. Mater.* (2022) 338, 111915

Programmable Nanosystems Through Chemical Pathways

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The powerful combination of chemical synthesis and self-assembly processes opened the path to create multiscale nanomaterials that mimic the complexity of those found in Nature. A natural evolution is taking place at high speed, from first generation nanomaterials with structure and morphology-controlled properties to *nanosystems*, in which properties can be programmed by precisely locating multiple functions in space. This second generation of complex nanoarchitectures with space-dependent properties can adapt to the environment and present dynamic and vectorial responses to stimuli.

Current efforts in this field are directed to produce *programmable nanosystems* with well-defined functional domains that can intercommunicate to obtain an *autonomous behaviour* derived from the local structure, the mesoscale architecture and the spatial location of different molecular, polymeric, biological or nanoscale functions.

Mesoporous materials (MM) constitute a highly tuneable platform for complex multiscale nanoarchitectures (i.e., molecular, mesoscale, macroscale...). Their pore symmetry and dimensions can be finely tailored, and “decorated” with a variety of molecular, bioactive or nanoscale components. Today, we can create truly programmable nanosystems, in which *confinement effects*, *responsivity*, or *collaborative functionality* can be imparted into the structure through the control of *positional chemistry* of different nanobuilding blocks.

We will present and discuss examples based in MM in which confinement, interaction management and localized reactivity are the basic topological toolkit that enables their construction and tuned properties. The combination and feedback of synthesis, characterization and modeling leads to pre-designed nanosystems with responsive and autonomous behaviour programmed in their structure at the molecular, mesoscopic and interfacial length scales. This set of concepts permits to build novel catalysts, enzyme cascade hosts, intelligent bioscaffolds, remotely activated nanoparticles, environment-responsive photonic crystals or perm-selective membranes.

The chemical strategies and tools at our disposal are key to design and produce a potentially infinite variety of programmable and intelligent matter with controllable behaviour, with wide applicability in bioinspired catalysis, environmental sensing, renewable energy, prosthetics, theranostics, soft robotics or synthetic biology.

Photonic applications of Organic-Inorganic Hybrids. From direction modulated photoluminescence to cellulose aerogels for environmental applications.

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Organic–inorganic hybrids (OIH) allow the fabrication of materials with tunable attributes offering modulated properties. In this talk we will show OIH featuring simultaneous iridescence and light emission^[1]. They are obtained through liquid crystal self-assembly of cellulose nanocrystal-template silica. The cellulose nanocrystal film structure comprises multi-domain Bragg reflectors and the optical properties of these films can be tuned through changes in the relative content of silica/cellulose nanocrystals. The incorporation of the light-emitting compounds allows a complementary control of the optical properties. The photonic structure plays the role of direction-dependent inner-filter, causing selective suppression of the light emitted with angle-dependent detection.

In the second part of the talk we will show new organic-inorganic hybrid aerogels based on bacterial cellulose. Composite Aerogels prepared from BC and photocatalysts like MoS₂, BiVo₄, BiOI and TiO₂ are proposed for decontamination of water through photocatalysis processes^[2-4].

Acknowledgements- Brazilian agencies CNPq, CAPES, FAPESP and the National Institute of Photonics (inct.info) are acknowledged for financial support

References

1. M.V.Santos et al, *Frontiers in Bioengineering and Biotechnology*, 2021, 9, 617328
2. L.Marchiori et al, <https://doi.org/10.1007/s10971-024-06380-2>
3. Silva et al, *ACS Appl. Mater. Interfaces*, 2023, 15, 23146
4. Santos et al, *Frontiers in Materials*, 2021, 8, 668835



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KEYNOTE LECTURES



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Polyoxometalate species as models of sol-gel metal oxide nanoparticles

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Polyoxometalates (POMs) represent an intriguing category of compounds, positioned between truly molecular species and nanoparticles. They typically possess a size just slightly larger than 1 nm (around 1.04 nm for the classic Keggin species $EM_{12}O_{40}^{n-}$, where E = P, Si, As, Sb, etc.) and carry a distinct electric charge. Studying their crystal structures alongside model amino acids and peptides as counter-ions helps illuminate the factors influencing the interaction between metal oxide nanoparticles and peptides/proteins. These factors include the hydrophilicity/hydrophobicity of the biomolecule ^[1], solution concentration and pH, and the presence of metal cations ^[2]. Additionally, the polarity of the M-O bond in POM species plays a crucial role ^[3]. While POM anions have limited basicity, in concentrated solutions with high acidity and trace amounts of highly charged cations, they can undergo protonation and sol-gel transition, forming self-assembled nanostructures ^[4]. These nanostructures hold significant potential as photo- and electrocatalysts due to the relatively high oxidative potentials of POM species.

Application of POM model particles permits even to visualize on molecular level the reaction mechanisms behind nanozyme activity of the metal oxide nanoparticles ^[5].

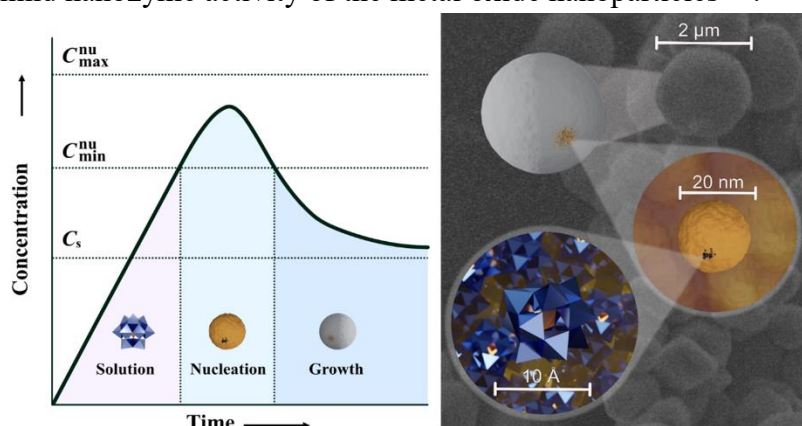


Figure 1. Formation mechanism of WO_3 nanostructure (spheres of spheres) produced by POM self-assembly.

References

1. B. Grejjer, T. De Donder, V.G. Kessler, et al. *Eur. J. Inorg. Chem.* (2021) 54.
2. B.H. Grejjer, G.A. Seisenbaeva, V.G. Kessler, et al. *Dalton Trans.* (2022) 51, 9511.
3. K.M. Rominger, G.A. Seisenbaeva, V.G. Kessler, et al. *Eur. J. Inorg. Chem.* (2019) 4297.
4. B.H. Grejjer, G.A. Seisenbaeva, V.G. Kessler et al. *Inorg. Chem.* (2024) 63, 3428.
5. A. Vanetsev, G.A. Seisenbaeva, V.G. Kessler et al. *Inorg. Chem.* (2024) 63, 8556.

Modulating textural and chemical properties in mesoporous organosilicas – the effect of addition sequence

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The combination of multifunctional organosilane precursors, self-assembly and control of the addition sequence of reactants provides an artist's palette of synthetic strategies that offer superb control over the textural and surface properties of silsesquioxane-based materials prepared via sol-gel processing. This presentation explores the formation of periodic mesoporous organosilicas (PMOs) obtained by the hydrolysis-condensation of organobridged triethoxysilane precursors in the presence of surfactants as structure-directing agents (SDAs)^[1]. After removal of the SDAs, the resulting materials usually exhibit monomodal, well-organized mesoporosity, with the size of the pores being controlled by the SDA. However, despite the potential applications of such materials with well-organized bimodal porosity, to the best of our knowledge, PMOs exhibiting two distinct types of ordered mesoporosity have seldom been described. Here, we describe a simple procedure for modulating the dimensions of ordered monomodal 2D hexagonal and bimodal porosity in PMOs synthesized from 1,4-bis(triethoxysilyl)benzene (BTEB) and Pluronic P123, by varying the addition sequence of reactants. The approach employs a single SDA without chemical or thermal degradation of the BTEB precursor. Reaction conditions leading to the formation of monomodal and bimodal porosity within the templated PMOs are identified. Our methodology exploits the competition between the rates of (a) BTEB hydrolysis/condensation; and (b) diffusion, solubilization and partitioning of the unhydrolyzed and hydrolysed precursor within the micelles. A mechanism describing the evolution of bimodal porosity within this system is proposed.

References

1. M. Laird, C. Carcel, E. Oliviero, G. Toquer, P. Trens, J.R. Bartlett and M. Wong Chi Man, *Microporous and Mesoporous Materials*, (2020) 297 110042.

Silicon polyolates: Opportunities and challenges in materials synthesis

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Organic silicon compounds are the key precursors in the synthesis of siloxane- or silica-based materials, like e.g. silicones, glasses or hybrid materials. Most frequently, alkoxy silanes based on monofunctional alcohols, such as $\text{Si}(\text{OR})_4$ or $\text{R}'\text{Si}(\text{OR})_3$ with $\text{R} = \text{CH}_3$ or C_2H_5 are used as starting compounds. Silicon polyolates, which can be obtained either from tetraalkoxy- / organotrialkoxysilanes or from biogenic amorphous silica with the corresponding polyols, have already been studied for many years. However they are still not very common in materials synthesis.

In this lecture, an overview of the rich diversity of the polyolate chemistry of silicon will be presented. Not only the structure and chemistry of these modified silanes, like e.g. tetrakis(2-hydroxyethyl)orthosilicate, bis(catecholato)silane or analogous carbohydrate derivatives will be highlighted, but also the differences in reactivity, e.g. hydrolysis and condensation reactions, in comparison to tetraethoxy- or methoxysilane will be discussed. However, these silanes offer far more interesting aspects, such as their role in diol or polyol-mediated de-polymerization reactions of (biogenic) silica towards a more sustainable route to $\text{Si}(\text{OR})_4$ or silica materials. In addition, utilizing diol- or polyol-based precursors in materials synthesis leads to novel opportunities regarding templated structures or processing strategies, e.g. 3D printing or melt-based syntheses.¹⁻⁷

References

- 1 S. Hartmann, D. Brandhuber, N. Huesing, *Acc. Chem. Res.* **2007**, *40*, 885-894.
- 2 C. Rosaria, R.M. Laine, M. Pagliaro, **2023** <https://doi.org/10.26434/chemrxiv-2023-qvz8z>
- 3 Luo, Qingqing, and Lutz Greb, *Europ. J. Inorg. Chem.* **2023** e202300186.
- 4 M.A. Brook, Y. Chen. K. Go, Z. Zhang, J.D. Brennan, *J. Mater. Chem.* **2004**, *14*, 1469-1479.
- 5 F. Putz. S. Scherer, M. Ober, R. Morak, O. Paris, N. Huesing, *Adv. Mater. Technol.* **2018**, *3*(7), 1800060.
- 6 Y. Chen, M.A. Brook, *Materials* **2023**, *16*. 2831.
- 7 T.G. Khonina, A.P. Safronov, M.V. Ivanenko, E.V. Shadrina, O.N. Chupakhin, *J. Mater. Chem. B*, **2015**, *3*, 5490-5500.

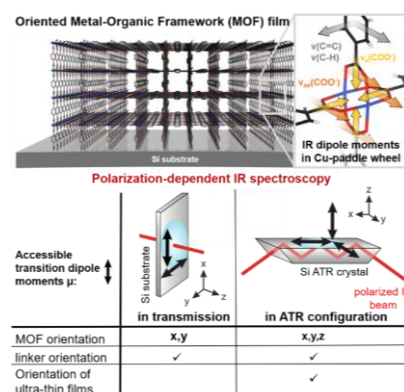
Infrared crystallography for evaluation of framework and linker orientation in metal-organic framework films

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In metal-organic frameworks (MOFs), organic linkers and metal-containing units are combined, forming porous materials with great variety and multiplicity regarding constituents' geometry, pore size and functionality. Their fields of applications are equally manifold and include photonics, energy-related applications such as solar or fuel cells, homogenous and heterogenous catalysis, gas and fuel storage, or (bio-)sensing. While MOFs are available in a great variety of shapes, such as nanocrystals, nanospheres, or hierarchical monoliths, The majority of these applications relies on the precise crystallographic orientation and uniform porosity of the MOF to allow for e.g. electron- or photoconduction. Hence, controlling and determining the crystallinity and orientation, including framework and linker orientation, of the MOF film with respect to the substrate is of prime importance for successful implementations. Recently, our group reported a synthetic method to obtain three-dimensionally oriented 2D and 3D Cu-based MOF films by epitaxial growth on copper hydroxide, yielding large scale films with controlled pore alignment.^{1, 2} Accessible approach to the structure of oriented MOF system is strongly required. X-ray diffraction is quite powerful tool to estimate crystal structure and orientation of thin film system. Especially, in-plane optical set up gives us a lot of information on the crystal structure and orientation parallel to the substrate. It is strongly required to establish an accessible measurement technique of structure and orientation of very thin MOF films. In this context, Fourier-transform infrared (FTIR) spectroscopy have several advantages: sensitive measurement for molecular system, accessible to many researchers, short acquire time and others. In this talk, evaluation of MOF framework structure and orientation using polarization-dependent FTIR spectroscopy is introduced.[4] Cu-based 2D MOF and 3D MOF films prepared via layer-by-layer method and from aligned Cu(OH)₂ substrates were studied with polarization-dependent FTIR spectroscopy in transmission and attenuated total reflection configuration as shown in Figure 1. The degrees of in-plane and out-of-plane orientation, the aromatic linker orientation and the initial alignment during layer-by-layer MOF growth, which is impossible to investigate by laboratory XRD equipment, was determined.^{3,4}



1. P. Falcaro, K. Okada, T. Hara, K. Ikigaki, Y. Tokudome, A. W. Thornton, A. J. Hill, T. Williams, C. Doonan and M. Takahashi, *Nature Mater.*, **16**, 342–348 (2017).
2. K. Okada, M. Nakanishi, K. Ikigaki, Y. Tokudome, P. Falcaro, C. J. Doonan and M. Takahashi, *Chem. Sci.*, **11**, 8005–8012 (2020).
3. B. Baumgartner, K. Ikigaki, K. Okada, M. Takahashi, *Chem. Sci.*, **12**, 9298–9308 (2021).
4. B. Baumgartner, R. Mashita, A. Fukatsu, K. Okada, M. Takahashi, *Angew. Chem. Int'l Ed.* **61** (28), e202201725 (2022).

Fig. 1: Cu-paddle wheel structure within an oriented MOF film. Transition dipole moments of the IR vibrations of the carboxylate and the aromatic ring present in the MOF are indicated with arrows. Schematic of IR spectroscopy in transmission and ATR configuration for thin film analysis and accessible transition dipole moments with respect to the surface.

Optimization of a synthesis procedure of nanocomposites silica/aliphatic polyesters by reactive extrusion for medical applications

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Aliphatic polyesters such as polylactide (PLA) and its copolymers (PLLA, PDLLA, PLGA) are booming materials due to their biodegradability, biocompatibility, and their biobased origin. First designed for medical applications, their interest for commodity applications has increased recently due to ecological regulatory constraints. However, their large scale adoption was faced to major technological challenges, in particular expensive costs of production and low mechanical properties for applications imposing high solicitations. To tackle to these two main issues, a reactive extrusion process was optimized to synthesize these aliphatic polyesters according to a rapid and continuous process. Adopting ring opening polymerization of cyclic monomers and combining a dried nitrogen atmosphere, an optimized screw configuration, and Sn(Oct)₂ and PEG (0.35 kDa) respectively as catalyst and protic initiator, this process allowed the synthesis of medical grade polyesters. After optimization of the processing parameters, this process permitted to reach high monomer conversion for poly-Llactide (*i.e.* > 98 %), poly-D,L-lactide (*i.e.* ~98 %), and poly-D,L-lactide-co-glycolide (*i.e.* ~94 %) with a final throughput of at least 100 g/h using a lab scale extruder. Although very fast and simple to perform, this method allowed the controlled synthesis of these polyesters in a large range of molecular weight [15-100 kDa].

Then, to meet the mechanical properties requirements of applications imposing high solicitations such as tissue engineering, nanocomposites silica/polylactide were optimized. To achieve homogeneous dispersion of filler inside the polymer matrix two main processing strategies were accessed: these composites were prepared either by *in situ* polymerization of lactide in presence of silica or by melt blending in extruder. Several approaches of chemical modification of silica surface were also applied to improve silica/polymer interactions: i) silanization of silica to anchor initiating sites for *in situ* lactide polymerization, ii) grafting of polylactide chains on silica surface either by “grafting from” or “grafting to” approaches. From this extensive study, the most appropriate methodology giving rise to nanocomposites relied upon 3 wt% silica pre-functionalized using the “grafting from” approach and using melt blending. Compared to neat PDLLA, this nanocomposite allowed an increase of around 100% and of 50% in Young modulus and ultimate tensile strength respectively.

Finally, the *in vitro* degradation kinetics of the PDLLA-silica composites were examined. Compared to neat PDLLA, the presence of silica enhanced the hydrolysis rate of PDLLA, especially when this inorganic filler was highly heterogeneously dispersed in polylactide.

Molecular Mechanism of Antimicrobial Activity of Tannins Through Joint Experimental and Computational Techniques

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Depletion of essential metal ions from the growth medium through chelation represents a likely molecular mechanism behind the antimicrobial activity of tannins. Indeed, with an increase in the growth medium concentration, MIC values of all investigated tannins rose roughly linearly in the case of *E. Coli*, while their relative order remained unchanged, indicating that a direct interaction of tannins with growth medium nutrients represents the likely source of their antimicrobial activity.^[1] Moreover, the generation times of *E. Coli* prolonged with increasing tannin concentration while the lag phase extended exponentially.^[2] Similar findings were obtained also for *Staphylococcus Aureus*.^[3] The UV/Vis spectra of gallic and ellagic acid pH dependence were predicted by TD-DFT methods and measured experimentally, which facilitated the determination of the stoichiometry and formation constant of the Fe(II)-gallic acid coordination compound through the Job plot construction.^[4] ^{5]} The deprotonation order and corresponding microscopic pKa values of 4 investigated ellagitannins were determined using ¹³C NMR spectroscopy as well as subsequently applied to elucidate the mechanistic model of the formation of their coordination compounds with Fe(II).^[6] Last but not least, the advanced ICP-OES technique was used to determine the amount of essential metal ions in *E. Coli* cells in the presence/absence of the investigated ellagitannins.

References:

1. S. Štumpf, G. Hostnik, M. Primožič, M. Leitgeb, J.-P. Samninen, U. Bren, *Molecules* (2020) **25**, 2947.
2. S. Štumpf, G. Hostnik, M. Primožič, M. Leitgeb, U. Bren, *Plants* (2020) **9**, 1680.
3. S. Štumpf, G. Hostnik, T. Langerholc, M. Pintarič, Z. Kolenc, U. Bren, *Plants* (2023) **12**, 2043.
4. G. Hostnik, J. Tošović, S. Štumpf, A. Petek, U. Bren, *Spectrochimica Acta Part A* (2022) **267**, 120472.
5. F. Frešer, G. Hostnik, J. Tošović, U. Bren, *Foods* (2021) **10**, 2689.
6. F. Frešer, U. Bren, G. Hostnik, *Spectrochimica Acta Part A* (2024) **313**, 124079.

Towards wearable (bio)chemical sensing with biocompatible functional nanomaterials

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This talk will present our current research on the development of optically sensitive (nano) materials and sensing schemes targetted at implementation on low-cost wearable devices. Design of wearable (bio)chemical sensors brings many challenges in device ergonomics, chemistry, physics, electronics, particularly for material/chemistry architecture which should ideally be reversible, reproducible and biocompatible [1].

Our research aims to adapt natural and biocompatible materials using appropriate chemical modifications to design optical sensing/sampling building blocks for integration with wearables. Initial work has focussed on wound and sweat monitoring [2], and an overview of optically responsive sensing chemistries for pH, electrolytes and redox active analytes designed for immobilisation on textiles and cellulose derivatives will be presented. Presently, our research efforts involve development of ionophore-based nanofiber optodes where the traditional plasticised PVC matrix is replaced by a biocompatible polymer, such as poly(ϵ -caprolactone) (PCL), plasticised with biocompatible citric acid esters (Figure 1).

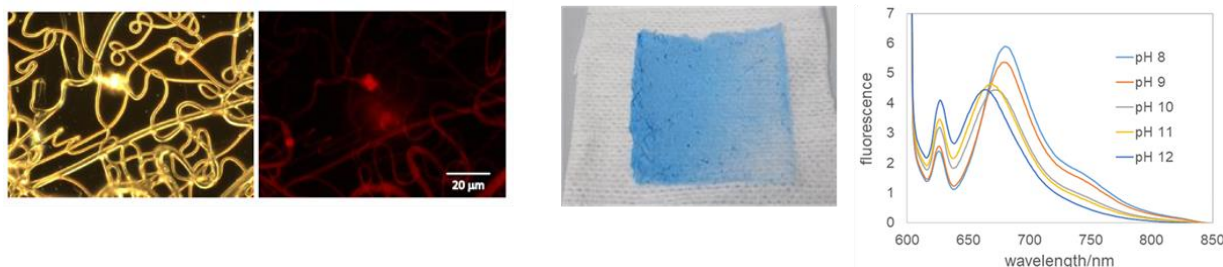


Figure 1. Nanofiber optodes obtained by electrospinning (microscopy images); electrospun layers on wound gauze material and fluorescence spectra at different pH

Lastly, the talk will introduce a new direction of research in which we intend to implement multimodal biomarker monitoring combining physical and biochemical parameters from the skin surface (on-skin patches) and under the skin (dermal tattoos) using wearable optoelectronic devices.

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References

1. M.D Steinberg, P. Kassal, I. M. Steinberg, *Electroanalysis* (2016) 28, 1149-1169
2. P. Kassal, M. Zubak, G.Scheipl, G. J. Mohr, M.D. Steinberg, I. M.Steinberg, *Sensors and Actuators B: Chemical* (2017) 246, 455-460

Advancing Scalability and Sustainability of Perovskite Nanocrystals Manufacturing for Photovoltaic and Optoelectronic Applications

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Metal halide perovskite nanocrystals (PNCs) have emerged as fascinating semiconductor materials for a wide range of optoelectronic applications encompassing lighting and displays, photovoltaics, solar-driven photo(electro)chemistry and photonics due to their exceptional optoelectronic properties. Compared to commercial photovoltaic and optoelectronic technologies, perovskite thin films can be processed on top of rigid and flexible substrates, at low-cost and low-temperature by using simple deposition techniques from PNCs solutions. Thus, they have been exploited to fabricate multicolour light emitting diodes (LEDs) and solar cells (SCs) with breakthroughs in the current state-of-the-art.

Despite significant advances, commercializing perovskite-based technologies requires finding up-scalable synthetic routes for high-quality PNCs with low defect density. Among many methodologies, microwave (MW)-assisted synthesis has proven to be a fast, easy, and sustainable way to produce PNCs. Microwave heating of the polar reaction mixture promotes highly homogeneous nucleation of perovskite seeds compared to the common hot injection method.

This presentation will cover the group's advances in MW-assisted synthesis of PNCs^[1-3], focusing on highly efficient LEDs based on CsPbX₃ (X: Cl, Br, I) colloidal nanocrystals. The energy consumption for MW fabrication compared to hot injection route will be discussed. Finally, the fabrication of alternative lead-free perovskite systems using this MW methodology will be presented. We are convinced that this technology is an outstanding and promising method towards more scalable and sustainable fabrication of perovskite-based materials.

References

1. T. C. A. da Silva, C. Fernández-Saiz, A. Gualdrón-Reyes, R. Sánchez, I. Mora-Seró, B. Julián-López, *J. Sol-Gel Sci. Technol.* **2023**. DOI:10.1007/s10971-023-06171-1
2. O. E. Solis, C. Fernández-Saiz, J. M. Rivas, D. Esparza, S.-H. Turren-Cruz, P. P. Boix, B. Julián-López, I. Mora-Seró, *Electrochimica Acta* **2023**, 439, 141701. DOI: 10.1016/j.electacta.2022.141701
3. E. Reyes-Francis, C. Echeverría-Arrondo, D. Esparza, T. López-Luke, T. Soto-Montero, M. Morales-Masis, S.-H. Turren-Cruz, I. Mora-Seró, B. Julián-López, *Chem. Mater.* **2024** 36, 1728-1736. DOI: 10.1021/acs.chemmater.3c03108

Design and synthetic approaches to hybrid adsorbents and bio-catalysts

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Solid adsorbents offer a promising alternative to enhance the sustainability of industrial separation and purification processes today. Key aspects in this pursuit involve recycling critical elements and purifying both wastewater and drinking water. Enhancing functionality necessitates tailoring of materials, employing appropriate supporting matrices and active ligand layers. Typically, for this purpose are applied hybrid materials, featuring an inorganic or biopolymer matrix, coated with grafted species that selectively bind to target components.

A major challenge in recycling critical elements is the separation of Rare Earth Elements (REE) from Late Transition Metals (LTM), particularly when LTMs are co-present in electronic, magnetic, and battery materials. The choice of an appropriate ligand function allows for the implementation of fundamentally distinct binding mechanisms for REE and LTM, thereby enhancing selectivity in both adsorption and, notably, desorption stages^[1-2]. Ligands that influence the oxidation states of LTMs may provide a means to separate individual constituents, such as Co and Ni, in components like the cathodes of Li-ion batteries^[3].

Among the challenges in water purification, two significant issues have emerged. One revolves around the accumulation of persistent organic pollutants (POP), notably pharmaceuticals. An effective, biocompatible, and soft chemical approach involves the oxidation of POP using biocatalysts, particularly peroxidase enzymes. However, preserving the activity of these enzymes necessitates their protection. As a sustainable solution, natural porous silicates like LECA, Perlite™, or silica gel derived from fly ash can serve as an encapsulation matrix for enzyme biocatalysts^[4].

Alternatively, purposefully constructed Metal-Organic Frameworks (MOFs) present another option for matrix material. These nanostructure supports have been synthesized through the structural transformation and exfoliation of MOFs composed of Rare Earth Element (REE) cations and asymmetric benzene-tricarboxylic acid. Enzyme molecules were adsorbed onto MOF nano sheets and integrated into microparticles through porous silica coatings^[5].

Per- or Polyfluorinated Organic Substances (PFAS) constitute another important kind of POP. PFAS concentrations are skyrocketing because of their earlier broad application in firefighting, cosmetics, clothing and food packaging. In our research we proposed application of complex polycationic functional layers with controlled hydrophilicity/hydrophobicity for their removal and accumulation^[6].

References

1. A. Vardanyan, G.A. Seisenbaeva, et al., *Nanomaterials* (2022) 12, 974.
2. T.C. Breijjaert, G.A. Seisenbaeva, et al., *Dalton Trans.* (2022) 51, 17978–17986.
3. M. Lakić, G.A. Seisenbaeva, et al., *Sep. Pur. Technol.* (2023) 323, 124487.
4. A. Vardanyan, G.A. Seisenbaeva, et al., *ACS EST Water* (2024) 4, 751–760.
5. O. Dudarko, G.A. Seisenbaeva, et al., *ACS EST Water* (2024) 4, 1303–1314.

Sustainable Processing of Innovative Rare-Earth Magnets

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The future of renewable energy and smart mobility depends upon permanent magnets (PMs), and those magnets depend upon Rare Earth Elements (REEs). From wind turbines and hydroelectric generators to electromotors in next-generation hybrid and electric vehicles, magnets are critical to Europe's future. The essential Critical Raw Materials (CRM) used in NdFeB PMs are REEs and non-REEs niobium and gallium. Although CRMs from China have been the primary source for Europe, supplies are uncertain, and the Chinese production chain is generally unsustainable. At the same time, the demand for REEs to make new PMs is projected to double in 15 years.

This work focuses on sustainable recycling and reproducing PM from sources of end-of-life (EOL) PMs focusing on the most common and readily available source of economically recyclable electric motors: home appliances. We are developing new dismantling and recovery procedures for PMs on highly available scrap and reproduction lines. We use an already well-established method of hydrogen in HPMS (Hydrogen Processing of Magnetic Scrap), followed by milling, degassing, and coating of sensitive powders. The first pilot experiments in producing bonded magnets out of recycled magnets confirm the no-waste circle economy processing and future independence from the unstable sources of REE.

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A novel approach in the use of bacterial nanocellulose for production of packaging films

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In the field of packaging materials currently synthetic polymer films made from oil based raw materials are the predominant material choice. While having good material properties, due to the fact that they are not biobased and biodegradable, their widespread use poses a growing challenge for the packaging industry, especially with new, stricter legislation on packaging materials being adopted. One of the potential solutions addressing these issues can be the use of nanocellulose, with its unique properties such as high strength, low density, high surface area and good barrier properties while being biobased and biodegradable.¹ It can be sourced either from fresh raw materials (e.g. wood cellulose) or from discarded side streams (bacterial nanocellulose produced with biotransformation). In terms of converting technologies, besides film forming 3D printing of polymer foils offers new possibilities in terms of developing new ideas and functionalities for packaging materials.² The aim of presented research was to develop nanocellulose foils with high (> 50 %) nanocellulose content made by 3D printing of nanocellulose hydrogels. The developed foils had homogeneous material composition and structure with adequate physical and mechanical properties. They were semi-transparent with non-glossy surface and relatively low water wettability.

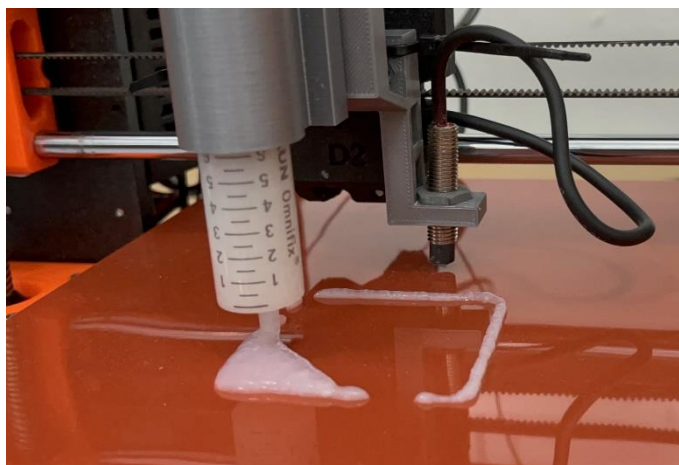


Figure 1. 3D printing system for nanocellulose.

References

1. R. Reshmy, E. Philip, D. Thomas, A. Madhavan, R. Sindhu, P. Binod, S. Varjani, M. K. Awasthi, A. Pandey, *Bioengineered* 12, 11463–11483.
2. R.B. Kristiawan, F. Imaduddin, D. Ariawan, Ubaidillah, Z. Arifin, *Open Engineering* (2021), 11, 639–649.

Nanocoatings from Biopolymers

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Biopolymers are synthesized naturally, conferring intrinsic advantages over synthetic polymers, such as biodegradability and biocompatibility. The former is essential for reducing the environmental impact of material waste, while the latter is critical for medical applications, including implants. Biomaterials can be used to prepare bulk materials or to coat other materials to modify their surface properties while preserving their bulk properties. For instance, biomaterial coatings can enhance the biocompatibility (e.g., hemocompatibility and cell interactions) of medical implants made from synthetic materials or metal alloys. They can function as drug carriers or be used as additives in nanoparticle coatings, aiding in coating deposition, fixation, and stability.

In this context, examples of biopolymers such as chitosan, hyaluronic acid, and others utilized as nanocoatings for medical implants and more will be discussed. The versatility of biopolymers in applications such as nanolayer or nanoparticle coatings, drug carriers, and coating additives will be demonstrated. Firstly, multilayers of oppositely charged cellulose polysaccharides were prepared on polycaprolactone films to enhance their resistance to blood-protein adhesion, a crucial factor in the initial stages of bacterial biofilm formation.[1] The assembly and subsequent protein interactions were analysed using a quartz crystal microbalance. The results indicated that increasing the number of layers heightened the hydrophilicity of the coatings, leading to improved protein repellence. Secondly, hyaluronic acid and chitosan nano- and microparticles were coated onto silicone surfaces to inhibit biofouling.[2] Nanoparticle formation was employed to incorporate antimicrobial agents and enhance adhesion to the silicone surface. The findings showed improved nanoparticle adhesion and antimicrobial activity. Thirdly, sulphated polysaccharide-coated magnetic nanoparticles were synthesized to enhance their hemocompatibility when used in the bloodstream. The sulphated polysaccharide coating resulted in reduced blood clotting, increased protein repellence, and improved cell compatibility. Lastly, cellulose-stabilized CaCO₃ nanoparticles were utilized to prevent acidic degradation of paper artifacts. The role of cellulose extended beyond particle stabilization to enhancing the migration of nanoparticles within the paper.

These studies underscore the significant potential of biopolymers in diverse applications, particularly in medical and environmental fields, where their unique properties can be harnessed to achieve superior performance and functionality.

- [1] M. Bracic, T. Mohan, R. Kargl, T. Grießer, T. Heinze, K. Stana Kleinschek, Protein repellent anti-coagulative mixed-charged cellulose derivative coatings, *Carbohydr. Polym.* 254 (2021). <https://doi.org/doi.org/10.1016/j.carbpol.2020.117437>.
- [2] M. Bračić, L. Fras-Zemljič, L. Pérez, K. Kogej, K. Stana-Kleinschek, R. Kargl, T. Mohan, Protein-repellent and antimicrobial nanoparticle coatings from hyaluronic acid and a lysine-derived biocompatible surfactant, *J. Mater. Chem. B.* 5 (2017). <https://doi.org/10.1039/c7tb00311k>.

Cellulose nanomaterials in innovative and emerging applications for sustainable and recyclable economy

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Cellulose nanomaterials (CNs) as renewable and bio-derived have received enormous scientific interest due to their abundance, easy manufacturing, biodegradability, and low cost, to address not only the technological challenges of sustainability and circularity but also social impacts. Such an interest also results from their unique properties, such as high mechanical strength, high degree of crystallinity, tunable shape, size, and functional surface chemistry, utilizing innovative technologies and applications.

This presentation will provide chemical and physical features of cellulose nanomaterials to be used as an adsorbent (heavy metals, dyes, bacteria; 1-3), an antimicrobial material (4), a functional material for barrier coating in textile (5-7) and paper packaging (8) industry, readily available filter membranes for water treatment or chromatographic supports for purification of biomacromolecules. Finally, their usage in advanced organic electronics (as dielectric film or el. conductor in energy-storage devices, 9) will be presented to replace thermoplastic polymers, while maintaining the devices` flexibility and lightness.

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References

1. Vivod V. et al., *Textile research journal* (2019) 89/6, 975-988.
2. Kokol V. and Vivod V., *Carbohydrate polymers* (2023), 318, 121134-14.
3. Kokol V. et al., *Membranes* (2023), 13/3 284-23.
4. Kokol V. et al., *Carbohydrate polymers* (2023), 311, 120603-16.
5. Kokol V. et al., *Cellulose* (2021) 28, 6545-6565.
6. Kolar T. et al., *Journal of industrial textiles* (2022), 51/5, 8267-8296.
7. Kokol V. et al., *Cellulose* (2021) 28, 6663-6678.
8. Ruberto Y. et al. *Cellulose* (2024), 31/6, 3589-3606.
9. Potta Thara Y.B. et al., *Cellulose* (2021), 28, 3069-3080. *New journal of chemistry* (2019) 43/2, 681-688.

Playing with the plasmonic properties of metal nanoparticles : single particles, colloidal self-assemblies and hybrid plasmonic glasses

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Metal nanoparticles possess unique optoelectronic properties that can be used in many processes and products, related to electronics, solar cells, biology and medicine and catalysis. Their synthesis processes still represent a challenge, in particular at large scale in view of their use in industry^[1,2]. The use of single object to tune the optical properties of hybrid materials will be developed^[3,4]. Introduction of chirality in such colloidal material is also an important challenge in optics. Recent work on synthesis of pentatwinned gold nanoparticles and their use as substrate for the growth of chiral particle will be discussed^[5]. Insight into the origin of chirality will be presented based on experimental and theoretical data. The control of colloidal assembly will be proposed to expand the properties range of the particles^[6,7]. Finally the preparation of hybrid plasmonic glasses for application in optical systems will be proposed^[8,9]. Experimental issues and challenges regarding the preparation and characterization of plasmonic glasses will be discussed.

References

1. D. Chateau, A. Liotta, F. Vadcard, J. R. G. Navarro, F. Chaput, J. Lermé, F. Lerouge, S. Parola, *Nanoscale* (2015) 7, 1934.
2. D. Chateau, A. Desert, F. Lerouge, G. Landaburu, S. Santucci, S. Parola, *ACS Appl. Mater. Interfaces* (2019) 11, 42, 39068.
3. S. Zaiba, F. Lerouge, A.-M. Gabudean, M. Iosin, J. Lermé, T. Gallavardin, O. Maury, C. Andraud, S. Parola, P. L. Baldeck, *Nano Letters* (2011) 11, 5, 2043-2047.
4. J. R. G. Navarro, F. Lerouge, C. Ceperaga, G. Micouin, A. Favier, D. Chateau, M. T. Charreyre, P. H. Lanoe, C. Monnereau, F. Chaput, S. Marotte, Y. Leverrier, J. Marvel, K. Kamada, C. Andraud, P. L. Baldeck, S. Parola, *Biomaterials* (2013), 34 (33), 8344-8351.
5. A. Carone, P. Mariani, A. Désert, M. Romanelli, J. Marcheselli, M. Garavelli, S. Corni, I. Rivalta, S. Parola, *ACS Nano* (2022) 16, 1089–1101.
6. Gold nanoparticles shape dependence of colloidal stability domains, A. Carone, S. Emilsson, P. Mariani, A. Désert, S. Parola, *Nanoscale Adv.* (2023), 5 (7), 2017-2026.
7. Colloidal assemblies of chiral plasmonic nanoparticles induce tunable circular dichroism response, A. Carone, P. Mariani, A. Désert, S. Parola, *Adv. Opt. Mater.* (2023), 11, 18, 2300119
8. D. Chateau, A. Liotta, H. Lundén, F. Lerouge, F. Chaput, D. Krein, T. Cooper, C. Lopes, M. Lindgren, S. Parola, *Adv. Funct. Mater.* (2016) 26 (33), 6005-6014.
9. D. Chateau, S. David, G. Berginc, C. Lopes, F. Chaput, F. Lerouge, A. Désert, C. Andraud, S. Parola, , *ACS Appl. Nano Mat.* (2022) 5, 3, 3773–3780.

Plasma nanofabrication for advanced SERS detection

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In the realm of plasmonic detection, pivotal for applications such as food and water quality monitoring, theranostics, and virus and toxin analysis, Surface Enhanced Raman Scattering (SERS) stands out as a powerful technique. Employing vibrational spectroscopy and surface nanoengineering, SERS leverages metallic nanoparticles to enhance signals through the confinement effect of the electromagnetic field, creating intense 'hot spots' near nanoscale metal surfaces. The morphology and arrangement of plasmonic nanomaterials crucially influence the formation of hot spot networks and signal enhancement factors of around 10^7 . This presentation focuses on our recent research in the plasma-assisted fabrication of advanced nanoplasmonic surfaces, showcasing nanocarbon structures, metal-oxide nano trees, and coupled nanogold. We demonstrate their versatility, reliability, and fast, one-step processing by utilising various plasma setups, including low-pressure and atmospheric pressure. These surfaces excel in detecting cancerogenic toxins at ppb levels, ultrafast recognition of trace chemicals, explosives, and even bacterial DNA detection with nanogram sample amounts. The talk underscores the significant potential of plasma-assisted nanofabrication in advancing nanoplasmonic surfaces for a broad spectrum of analytical applications.

References:

1. V. Shvalya, G. Filipič, J. Zavašnik, I. Abdulhalim & U. Cvelbar, *Applied Physics Reviews* (2020) 7(3), 031307.
2. M. Santhosh, N., Shvalya, V., Modic, M., Hojnik, N., Zavašnik, J., Olenik, J., Košiček, M., Filipič, G., Abdulhalim, I. & Cvelbar, U. *Small* (2021) 17(49), 2103677.
3. V. Shvalya, A. Vasudevan, M. Modic, M. Abutoama, C. Skubic, N. Nadižar, J. Zavašnik, D. Vengus, A. Zidanšek I. Abdulhalim, D. Rozman & U. Cvelbar, *Nano Letters* (2022) 22 (23), 9757-9765.

Characterisation of thin films and nano-layered composite materials by photothermal techniques

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Photothermal techniques such as photothermal beam deflection spectroscopy (BDS) and thermal lens spectrometry (TLS) provide unique analytical tools for materials' characterization, which enable non-contact and non-destructive determination of thermal and optical properties, such as thermal conductivity, thermal diffusivity and spectral characteristics. In case of BDS some properties related to thermal parameters can be determined as well (i.e. porosity, surface roughness, charge carrier lifetimes). Furthermore, BDS enables dept profiling and studies of sub-surface structures and distribution of thermal properties or even compounds in composite materials, which can be achieved by scanning the amplitude and phase of photothermal signal generated over a wide range of excitation modulation frequencies (Hz -100 kHz).

In this presentation the basics of photothermal spectroscopy and related instrumentation will be presented, while the principles of operation will be illustrated by practical applications of photothermal techniques for characterisation of nanostructured materials. These will include optical and structural characterization of thin layered photocatalysts^[1], demonstration of plasmon assisted luminescence on gold nanoislad films^[2], determination of heat-transfer properties of nanodiamond solutions^[3], dept profiling of drug distribution in aerogel composites for coatings of medical implants^[4], and others.

References

1. D. Korte, M. Franko et al., *Opt. Mater.* (2015) 42, 370-375.
2. H. Cabrera, M. Franko et al., *Talanta* (2018)183, 158–163.
3. M. Proskurnin et al., *J. Phys. Chem. C* (2021) 125, 7808–7823.
4. M. Bračič, M. Franko et al., *Appl. Surf. Sci.* (2023) 611, 155621.



NANOAPP 2024

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INVITED LECTURES



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AI and data throughout circular textile flow

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The presentation will provide insights into the development of AI and its current applications in textile supply chains. Furthermore, the presentation will examine the implications of circular economy principles on data needs, exploring how the shift towards circularity impacts data collection, analysis, and utilization. Key issues to be addressed include the challenges and opportunities presented by integrating AI with circular practices, the necessary technological advancements, and the potential benefits for the textile sector. The presentation will also introduce the EU project PESCO-UP, detailing its objectives, ongoing research, and expected contributions to advancing AI and circularity in textile supply chains. This will help attendees understand the project's role in driving industry transformation and promoting sustainable practices.

Enhancing Personal Protective Equipment Waste Recycling: A Comprehensive Analysis of Polymer Recyclates from Disposable Surgical Masks

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The production of personal protective equipment (PPE) has surged significantly in recent years, driven not only by the pandemic but also by stricter employee protection regulations [1]. According to different analytical groups, the PPE market will still grow significantly in the following years [2,3]. The increased use of PPE, particularly disposable surgical masks (DSMs), is placing additional demands on waste management systems and causes environmental pollution when it is not treated correctly [4]. Consequently, developing high-quality solutions for managing this type of waste is crucial. Although mechanical recycling remains the predominant method, the resulting recyclates are often considered low-grade materials. Therefore, a comprehensive analysis of these recyclates is essential [5]. This analysis will help us enhance their properties and identify appropriate end-use applications to increase their value.

This study extensively analyses recyclates derived from DSMs made of various polymers. Through surface and morphology tests, we have gained insights into the distribution of different polymers within polymer blends and their impact on mechanical and surface properties. The results indicate that incorporating ear loop material into the polypropylene (PP) melt enhances the toughness of the material. In the resulting polymer blends, PP and polyamide 6 (PA 6) dominate the surface, influencing surface properties, while polyurethane (PU) and polyethylene terephthalate (PET) are primarily distributed within the injection-molded samples.

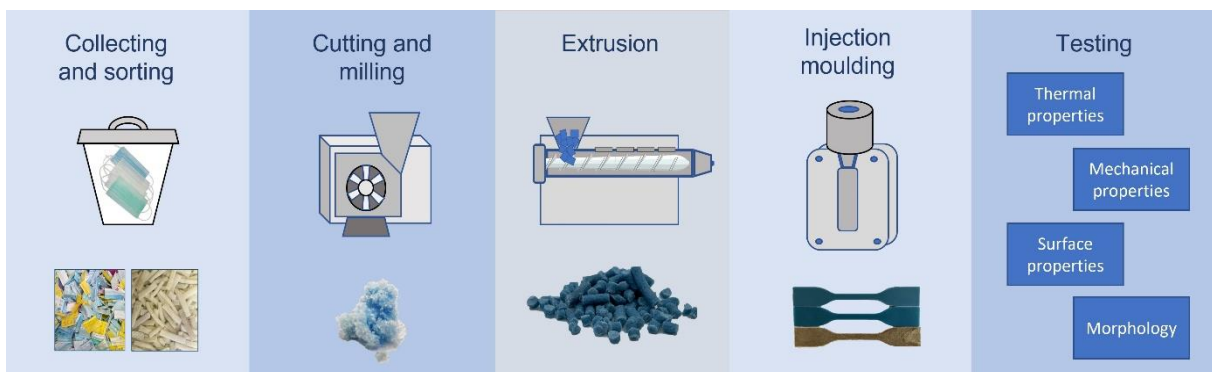


Figure 1: Mechanical recycling proces of DSM from collecting to testing

References

1. Remic, K., et al., *Public Handling of Protective Masks from Use to Disposal and Recycling Options to New Products*. 2022, 2022. **68**(4): p. 9.
2. Dive, R., *Disposable Protective Clothing Market by Type (Polypropylene, Polyethylene, Polyester, and Others), Application (Chemical, Biological, Mechanical, Thermal, and Others), End-use (Healthcare, Manufacturing, Food Processing, and Construction), and Regional Analysis (North America, Europe, Asia-Pacific, and LAMEA): Global Opportunity Analysis and Industry Forecast, 2021–2028*. 2020.
3. Markets, M.A., *Market Reports. Personal Protective Equipment Market by Type (Hands & Arm Protection, Protective Clothing, Foot & Leg Protection, Respiratory Protection, Head Protection), End-Use Industry (Manufacturing, Construction, Oil & Gas, Healthcare) - Global Forecast to 2022*. 2022.
4. Erjavec, A., et al., *Significant Fragmentation of Disposable Surgical Masks—Enormous Source for Problematic Micro/Nanoplastics Pollution in the Environment*. *Sustainability*, 2022. **14**(19): p. 12625.
5. Erjavec, A., et al., *Advance Analysis of the Obtained Recycled Materials from Used Disposable Surgical Masks*. *Polymers*, 2024. **16**(7): p. 935.

Towards secondary raw materials

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Every year across the world we produce 92 million tonnes of textile waste. Unless big changes happen and improve how we make, use, and dispose of clothes, it's estimated that by 2030 we'll create 134 million tonnes of textile waste globally. In Europe, around 15 kg of textile waste is generated per person every year, among which post-consumer waste (discarded clothes and home textiles) represents 85%¹. Only about one quarter of this amount (4.4 kg) was collected separately for reuse and recycling, but the rest ended up in mixed household waste² and eventually at the landfills or in incineration plants.

The significant transformation is the only way to mitigate the negative consequences to environment and people. Reduction of overproduction and overconsumption, the extension of product life time and designing products for increased circularity would contribute significantly, however the recycling is unavoidable to create the complete solution. Four main technology archetypes: mechanical, thermo-mechanical, chemical and thermos-chemical recycling cover a series of textile recycling technologies that have the potential to jointly recycle 70 % of EU textile waste into fibres (closed loop applications)¹. Considering raw material composition cotton represents the majority (58%), followed by polyester (30%), man-made cellulose (5%) and polyamide (3%) and wool (1,2%)³.

In the paper we aim to present the textile and packaging (bio)chemical recycling concept, developed within IOS's past and recent R&D activities. This includes scaling up all process steps (recognition, sorting, pretreatment, degradation, post-treatment) from basic experimental work at lab scale, over proving the concept at the demo pilot plant to finally designing the equipment and processes for industrial environment. The concept combines chemical and biochemical approaches aiming to result in trade-off between recycling the polyester and cellulosic waste through energy (cost) effective process and a process that yields in virgin (market-acceptable) quality of secondary raw materials (chemicals).

The presented R&D work is supported by ongoing EU projects:

OpenLOOP (190115848-OpenLOOP-HORIZON-EIC-2022-ACCELERATOR-01), **PESCO-UP** (101138367-PESCO-UP-HORIZON-CL4-2023-TWIN-TRANSITION-01) and **MixMatters** (101112409-MixMatters -HORIZON-JU-CBE-2022).

References

1. Scaling textile recycling in Europe—turning waste into value, McKinsey&co, Apparel, Fashion & Luxury Group, July 2022
2. European Environmental agency (EEA), 2024
3. Material Change Index Insights 2022, Textile-Exchange_MCI-Insights_2022.pdf

Piloting and scaling-up textile recycling – challenges, solutions and opportunities

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Currently only 1% of the clothes that are used are recycled into new clothes. The cycle from clothing to waste is also fast – 60% of the manufactured clothing ends up in the landfill within one year of its manufacturing date. Textiles has been called as one of the world's least sustainable industry and the fashion industry is estimated to be responsible for 10% of global CO₂ emissions, which is more than international flights and maritime shipping together!

Valmet is a leading global developer and supplier of process technologies, automation and services for the pulp, paper and energy industries. We believe that the proven solutions and knowhow in fiber treatment processes can be adjusted to evolving textile fiber processes and therefore, are keen to explore new business opportunities in textiles; both in fiber-to-fiber recycling and novel man-made cellulose fibers (MMCF). Valmet's overall target is to develop and commercialize novel process concepts and related equipment with the technology owners.

Piloting and up-scaling are areas where Valmet is keen to offer its solutions. Through our experiences we have identified some challenges, but also solutions and opportunities in the field of textile recycling.

One of the challenges relates to the complex raw material in textile recycling, which is often a combination of natural and synthetic fibers intertwined and not easily separated. Processing of natural fibers is more known to Valmet and we have to come up with innovative solutions on how to recycle also the synthetic part, in a value-added and reusable manner. This leads to one of the opportunities in the field, which is the innovative start-up scene. Technology providers, such as Valmet, need to work in close collaboration with these technology owners and support them in scaling up their processes. One of the solutions to tackle the recycling challenge is thus collaboration – actions and investments are needed from all the actors in the value chain.

In this presentation, I will highlight the challenges and opportunities as well as the solutions related to textile recycling, from the perspective of Valmet.

Recycling of cellulose materials

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Textiles containing cellulose (cotton) and cardboard/carton waste represent a significant reservoir of untapped organic carbon. These wastes have enormous potential as carbon feedstock in industrial biotechnological processes. Essentially, cotton/cardboard (CC) waste is pure cellulose (with some additives) in the form of polymerized glucose consisting of β -(1 \rightarrow 4)-linked D-glucose subunits. One of the largest and most diverse classes of natural chemicals that can be produced from glucose are terpenes, which have a wide range of applications as flavours, fragrances, pharmaceuticals, biopesticides, and biofuels. Here, we have investigated the bioconversion of CC waste into the exemplary terpenes such as limonene or cineol as a proof of concept. using the *Escherichia coli* (*E. coli*) as microbial cell factory. The D-glucose was metabolized via a manipulated heterogeneous biolipid synthesis pathway (the mevalonate pathway) introduced into *E. coli* to produce those compounds. Additionally, we have developed a novel strategy of producing and capturing these highly volatile chemicals by growing *E. coli* on solid medium, termed solid state production (SSP). The SSP strategy to produce volatile value-added chemicals represents an important proof of concept for the production of terpenes from hydrolyzed CC waste streams.

The role of lanthanides and dyes in enhancing the photoluminescence of silica sensors for pharmaceutical monitoring in water

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Our research focused on analyzing the photoluminescence spectra of aqueous suspensions of synthesized silica particles to uncover further potential applications. This analysis has revealed a strong photoluminescent response in these particles, underscoring their potential as versatile sensors capable of detecting pharmaceuticals in various environmental settings. Such technological advancements are crucial, as modern pharmaceutical applications demand sophisticated sensors to ensure public and environmental health. The silica sensors, equipped with lanthanides and dyes, demonstrate exceptional sensitivity, vital for integrating nanotechnology with pharmaceutical testing across diverse settings.

This study has developed and tested novel sensors using silica particles tailored with amino and other hydrophobic groups such as phenyl or thiol, which are aimed at environmental and biochemical sensing. Significant findings include the creation of a luminescent sensor using Rhodamine 6 G-modified silica particles, which effectively detect carbamazepine in sewage water, showcasing a wide detection range. Additionally, we synthesized a nanosized adsorbent from quartz modified with diamino and phenyl groups that exhibits high sorption efficiency for lanthanides from battery waste, enabling the detection of doxycycline in water. Moreover, spherical particles with thiol and amino modifications, combined with Eu(III) or Fluorescein, display strong photoluminescence when exposed to oxytetracycline or norfloxacin, respectively, demonstrating their versatility as sensors. By enhancing the photoluminescence properties of these particles, we have significantly improved their application in environmental and healthcare monitoring, contributing to the detection and analysis of complex pharmaceutical compounds.

This research is funded by APVV-19-0302, VEGA 2/0138/24, Štefan Schwarz Postdoc Fellowship No. 2023/OV1/016, HORIZON-MSCA-2022-SE-01 №101131382 project, and the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project 09I03-03-V01-00098.

Electrical sensitization of magnetic nanoplatelets

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A rare example of a ferrofluid (FF) composed of permanently magnetic nanoparticles is based on barium hexaferrite nanoplatelets (BHF NPLs). In contrast to classic FFs consisting of superparamagnetic nanoparticles, the BHF NPLs are ferrimagnetic with a substantial remanent magnetization. In the first FFs, the BHF NPLs were dispersed in alcohols. From those, the first ferromagnetic liquids were developed ^[1]. Due to high sensitivity to a magnetic field and significant magneto-optic effect, the BHF NPLs FF can be used in a variety of sensors, such as magnetic-field sensors ^[2]. The second generation of the BHF NPLs FF is based on apolar solvents that enable their application in an electric field. We will present examples of various BHF NPLs FFs and their physico-chemical properties. Moreover, we will show that the BHF NPLs can be electrically sensitized to form a magneto-electric liquid ^[3].

References

1. A. Mertelj, D. Lisjak, M. Drofenik, M. Čopič, *Nature* (2013) 504, 237.
2. V. Budinski, S. Pevec, S. Čampelj, A. Martelj, D. Lisjak, D. Đonlagić, *Opt. Lett.* (2022) 47, 4696.
3. D. Lisjak, A. Mertelj, A. Tufani, S. Čampelj, T. Landovsky, V. Novotná, M. Cigl, Magnetolectric liquid: EPEP24170316, 2024-04-15. München: European Patent Office, 2024.

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Ceria-Based Nanocomposites for Catalysis by Magnetic Heating

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Conversion of (renewable) electricity into fuels and chemicals, i.e., the electrification of chemical industry, is one of the keys for decarbonising the planet. Catalysis by magnetic (also referred to as induction) heating is an emerging technology, which enables the efficient use of electricity to supply the heat for thermo-catalytic processes. The technology is based on heating of magnetic nanoparticles imbedded in a catalyst support in an alternative magnetic field. The selective heating of catalyst surfaces can improve the selectivity and yields of catalytic reactions. In addition, the technology is very flexible (very fast heating and cooling rates) and brings high hopes for improving energy efficiency.

In this study, magnetic ceria-based catalysts were synthesized. First, magnetic iron-oxide nanoparticles were coated with nanocrystalline ceria using controlled precipitation of the Ce³⁺ ions in the presence of hexamethylenetetramin (HMTA) in the aqueous suspension. In the next step, Ru catalytic nanoparticles were deposited onto the magnetic ceria support. A special attention was given to reveal chemical mechanisms enabling the deposition of homogeneous ceria coatings with a high surface area. Morpho-structural properties of the synthesized materials were characterized using a combination of electron microscopy (SEM, TEM, and aberration-corrected STEM), measurements of specific surface area (BET) and XRD. The efficiency of magnetic heating was evaluated as a function of the amplitude of magnetic field and the structure and magnetic properties of catalyst (measured with VSM). Finally, the magnetic catalysts were tested for relevant chemical conversions where the magnetic heating was compared with the conventional heating.

Implementing a supportive environment for lifelong learning for sustainable engineering (Green2Eng)

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The impact of society on the environment has become extremely threatening, especially in recent decades. Therefore, society and each and every one of them must become environmentally aware in order to fulfill their responsibility for the environment and ensure sustainable development. A green transition in society will only be possible if we invest in knowledge that leads to solutions that are efficient and consume less energy. The basis of technological development is experts in science and technology, which increases the demand for knowledge and skills for environmentally conscious, sustainable engineering. Engineering and science education must be based on transdisciplinary teaching and learning strategies that incorporate the content and interdisciplinary approaches of environmentally conscious, sustainable engineering in addition to the basic, narrow disciplinary knowledge and skills within each science so that future experts (students) and non-experts (individuals not enrolled in higher education) develop critical thinking and environmental awareness from which they can create sustainable products, programs and solutions. To address this gap and ensure skills are adequate for new technologies, additional education or requalification is essential. Various forms of training, such as short or long courses, independent study, and internal supplementary education, are available, though these are not systematically regulated. One effective method to quickly and efficiently bridge this knowledge gap in the field of new technologies is the introduction of micro-credentials.

This conference paper discusses the initiatives of the European Union and the Slovenian government to support the development, implementation and mutual recognition of micro-credentials between institutions, companies and sectors in Slovenia and the EU. Micro-credentials facilitate lifelong learning, which is crucial for equipping individuals with the necessary knowledge, skills and competences for personal and professional success. The Faculty of Mechanical Engineering at University of Maribor is one of the partners in introducing best practices from the field of lifelong learning in the development of short courses and their further development into micro-credentials, which will then be used to build a national platform for micro-credentials through joint actions of the University of Maribor, other Slovenian universities and the relevant ministries.



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ORAL LECTURES



Advancing Mercury Detection: A MerB (Organomercurial-lyase)-based Solid-State Voltammetry Sensor for Methylmercury detection

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Mercury is a highly toxic and mobile element that has had a pronounced and adverse effect on organisms. Accordingly, bacteria have evolved mer operons to meliorate the toxic action of different chemical forms of mercury. The bacterial mercury detoxification system contains two proteins, organomercurial lyase (MerB) and mercuric ion reductase (MerA). MerB specifically catalyses the protonolysis of the carbon-mercury bond of methylmercury (MeHg), resulting in the formation of a reduced carbon compound and inorganic ionic mercury (Hg^{2+}) [1]. We intend to develop a simple solid-state voltammetry sensor for detecting MeHg through changes in the current across gold films caused by the redox potential of Hg-bound-MerB (Organomercurial lyase) after cleaving MeHg. Since MerB is a highly specific organomercurial lyase, we plan to use its Met-Hg-specific binding characteristics as a sensing/receptor component of the sensor. On binding of MeHg onto MerB, the current fluctuation in the conductive paths ultimately percolates the entire gold film [2]. To achieve that, we have prepared an expression system that will enable us to obtain enough highly active MerB enzymes. The expressed MerB enzyme with his-tag was purified and it showed High Hg-bound onto the MerB after cleaving from MeHg for preparing the Met-Hg-specific sensor. For the reporter system, We would prepare an SPE (Screen-printed gold electrode) and functionalize with thiol followed by NTA-Ni²⁺ (Nitriloacetic acid with Nickel) for specific Histag MerB proteins binding.

References

Gregory C. Benison, Paola Di Lello, Jacob E. Shokes, Nathaniel J. Cospers, Robert A. Scott, Pascale Legault, and James G. Omichinski. (2004). *Biochemistry* 43(26), 8333–8345.

Eun Seon Cho, Jiwon Kim, Baudilio Tejerina, Thomas M. Hermans, Hao Jiang, Hideyuki Nakanishi, Miao Yu, Alexander Z. Patashinski, Sharon C. Glotzer, Francesco Stellacci and Bartosz A. Grzybowski. (2012). *Nature Mater* 11, 978–985

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Recycling of textile wastes – EIC OpenLOOP project

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Recycling of various wastes is a critical topic, with emerging technologies for the chemical and enzymatic recycling of textile and plastic wastes. However, to date, no significant industrial plants have been constructed for the recycling of PET and cellulosic textiles or plastics. The OpenLOOP project aims to bridge this gap by efficiently addressing textile recycling. The project encompasses the treatment of not only textile blends but also pure streams of cellulose and PET simultaneously. With a DEMO plant designed for recycling pure PET, pure cellulose, and Cell/PET mixtures, we aim to address over 90% of all textile waste. The same reactors can also be adapted for PA 6 depolymerization, targeting an additional 2% of total textile waste. However, other polyamides (PAs) are not the focus of this SME project due to the problematic and costly separation processes required. Mixed (and pure) plastic/cellulose waste poses a substantial environmental challenge, as demonstrated by textile waste composed of blended fibers. Without viable recycling strategies, Europe disposes of 75% (4.3 million tons) of its textile waste annually. Current strategies either postpone the issue (reuse) or provide temporary solutions (mechanical recycling). Eventually, textile waste becomes non-recyclable and ends up either incinerated (expensive and only provisionally sustainable) or landfilled (unsustainable). A promising new approach is emerging in the form of chemical recycling technologies like OpenLOOP, which degrade waste back into building-block chemicals, allowing for virtually infinite reuse. Despite its potential, the uptake of chemical recycling remains low. OpenLOOP offers a novel chemical recycling technology that:

- Can degrade any mixture and blend of PET (polyethylene terephthalate) plastic and cellulose waste.
- Produces high-value feedstock, including 5-HMF (5-hydroxymethylfurfural), LA (Levulinic acid), furfural, and rTA (recycled terephthalic acid).
- Is environmentally friendly, using only water and clean processes, and can be successfully implemented in an industrial environment.

In OpenLOOP, we aim to advance the technology, integrate it into industrial settings such as IOS's DEMO plant, automate procedures for safety and simplicity, validate the technology, engineer process steps for optimal productivity, design commercial packages, develop the supply chain, and enter the market.

Advanced regenerated cellulose materials for emerging applications

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Owing to increasing global ecological concerns about environmental pollution from petrochemical-based materials and the associated sustainable development policies, there is an indispensable need and demand for utilizing eco-friendly components derived from renewable resources in the R&D of new, more sustainable materials and fabrication systems^{1–3}. Cellulose, as the most abundant renewable polymer and green biomass resource on Earth, can be obtained from a vast array of sources such as the cell walls of wood and plants, certain species of bacteria, algae, and tunicates^{2,4,5}. It has drawn significant attention due to its wide availability, low cost, biocompatibility, biodegradability, thermal and chemical stability, derivatizability, etc². Interestingly, the cellulose can be regenerated through its dissolution and re-generation processes using solvents and anti-solvent reagents, respectively⁶. This presentation focused on developing various types of regenerated cellulose (RC) materials, including all-cellulose composites (ACCs), 3D bio-printed RC filaments, dry-jet wet spun RC fibers, as well as prototypes of RC films and RC-based bionanocomposites (BNCs) using ‘green’ solvent systems. Specifically, a notable research effort was elucidated on developing pure silica-fiber textiles and biocomposite structures produced from wet-spun RC fibers, aimed at hard tissue engineering applications. Additionally, an interesting study was presented on the development of surface-functionalized RC fibers for their heat retention and release characteristics, targeting applications in emotional clothing and exploring further applications for far-infrared activity in biomedicine. The current and potential applications of each demonstrated RC material were specified, alongside presentations on the potential development of other forms of RC materials, including hydrogel, aerogel, cryogel, xerogel, membranes, and more.

References

1. Bhattacharjee, M., Dhar, A. & Sikdar, P. Recent Advances in Regenerated Cellulosic Materials and Composites for Multifunctional Applications: A Review. in *Regenerated Cellulose and Composites* (ed. Shabbir, M.) 37–78 (Springer Nature Singapore, Singapore, 2023). doi:10.1007/978-981-99-1655-9_3.
2. Wang, S., Lu, A. & Zhang, L. Recent advances in regenerated cellulose materials. *Progress in Polymer Science* **53**, 169–206 (2016).
3. Yapar, Ö. 3D Bioprinting of Cellulosic Structures for Versatile Applications. in *Additive Manufacturing in Multidisciplinary Cooperation and Production* (eds. Drstvensek, I., Pal, S. & Ihan Hren, N.) 79–102 (Springer International Publishing, Cham, 2024). doi:10.1007/978-3-031-37671-9_8.
4. Shen, H., Sun, T. & Zhou, J. Recent Progress in Regenerated Cellulose Fibers by Wet Spinning. *Macro Materials & Eng* **308**, 2300089 (2023).
5. Seddiqui, H. *et al.* Cellulose and its derivatives: towards biomedical applications. *Cellulose* **28**, 1893–1931 (2021).
6. Zainul Amir, N. A. *et al.* Regenerated Cellulose Products for Agricultural and Their Potential: A Review. *Polymers* **13**, 3586 (2021).

Plasma-Modification of graphene oxide for advanced ammonia sensing

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Reduced graphene oxide (rGO) is currently studied for its excellent tailorability, which enables its use in gas sensing applications. The reduction of graphene oxide (GO) can be achieved through various methods, with plasma treatment standing out as a green and rapid approach. This study introduces a controlled plasma-based process for the swift and environmentally friendly reduction of GO films, optimized for detecting ammonia (NH₃) at room temperature in ppm concentrations. We drop-casted GO on copper electrodes and then employed a mild hydrogen plasma treatment to tune the sensitivity and reversibility of the sensor. The experiments were conducted in a low-pressure hydrogen plasma at 100 W, with treatment durations ranging from 10 to 240 seconds. Structural and chemical analyses indicated a rapid decrease in oxygen content from approximately 30% to 20% within the first 20 seconds of treatment. We examined the impact of different treatment durations on sensitivity and recovery. The sensor treated for 20 seconds ('rGO - 20 s') exhibited the highest sensitivity, detecting NH₃ at 23.9% (100 ppm) and 47.1% (1049 ppm). However, this increased sensitivity came with a trade-off: a recovery time roughly four times longer than that of the sensor treated for 240 seconds ('240s-rGO'). This variation is attributed to the distinct interactions between NH₃ and rGO, which are dominated by chemisorption and physisorption.



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Amino-Modified Iron Oxide Nanoparticles for Efficient Adsorption of Cu(II), Fe(III), Co(II), and Cd(II) Ions from Water Solutions

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Testing and validating adsorption efficiency of the individually designed functional (magnetic) nanomaterial is more than ever in focus, to meet the requirements for water reuse and heavy metals recycling nearing Circular economy. [1] In compliance with the CRM Act Regulation and recently updated EU CRM list (2023), all raw materials, even if not considered critical at the moment (i.e. Iron, Cadmium and Copper), are nowadays important for the EU economy. [2] Moreover, the prognosed shortage of specific HMs (i.e. Cobalt) the industry by 2050, is currently the driving force for the development of technologies for recovery and reuse. [3] Unlike other technologies, adsorption process enables the adsorption and recycling of both the adsorption material itself and the adsorbed substances, while practically no other method enables this. Adsorption has become very popular, due to the possibility of using different adsorption materials and simple implementation. [4] In order to enhance circularity and improve recycling of heavy metal ions many designed nano, magnetic and amino-functionalized nanoparticles show potential for removal of critical and valuable HMs from water solutions, contaminated and industrial wastewater. [5] However, prior using any newly designed magnetic nanoparticles (MNPs) in real environment, adsorption process needs systematically approach in order to define and validate optimal conditions for removal of targeted HMs from water environment. [5]

In this work circular economy approach – the adsorption process and desorption of heavy metal (HM) ions —i.e., copper (Cu²⁺), iron (Fe³⁺), cobalt (Co²⁺) and cadmium (Cd²⁺) were tested. Synthesized amino-modified iron oxide MNPs (γ -Fe₂O₃@NH₂ NPs) were tested for specific and selective adsorption, reuse and desorption of HMs from acidic (pH=4) and neutral aqueous solution (pH=7). Amino-MNPs were characterized by TGA, FTIR, TEM / EDXS, and zeta potential. Adsorption was tested on optimal adsorbent amount ($m_{ads}=45$ mg) as revealed in our previous extensive research [6], and desorption cycle proven with 0.1 M HNO₃ for material adsorbed in acidic and in alkaline solution. Kinetic modelling for adsorption process at pH=7 was also done.



We obtained improvement of adsorption efficiency and capacity for copper (Cu^{2+}), iron (Fe^{3+}) ions at pH 7 without any pretreatment by 45 mg $\gamma\text{-Fe}_2\text{O}_3\text{@NH}_2$ NPs. Less exciting were results for other ions. Efficiency order: Cu^{2+} (99,5%) > Fe^{3+} (99,9%) after 1min > Co^{2+} (26,9%) > Cd^{2+} (19,8%)/30 min, with the corresponding adsorption capacities 98,8 mg/g, 80,3 mg/g after 1 min, 18,3 mg/g and 16,8 mg/g after 30 min, respectively. The kinetic modelling indicates covalent binding of Fe^{3+} , Co^{2+} and Cu^{2+} ions and the diffusion of Cd^{2+} ions to the surface of the magnetic adsorbent. Results show also potential for iron (Fe^{3+}) ions at pH=4, while less appropriate for other ions. In fact, the desorption results (for Cd^{2+} (97,7-99,9%) > Cu^{2+} (89,2-99,9%)) show the possibility for reuse of $\gamma\text{-Fe}_2\text{O}_3\text{@NH}_2$ NPs with 0,1 M HNO_3 , but development of the adsorption system and retention of MNPs for application in real water treatment remains challenging and needs improvement.

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The results were also created within the Research program Design of new properties of (nano)materials & applications, No. P2-0424 and research project No. Z2-4483. The authors acknowledge the financial support from the Slovenian Research Agency.

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References:

1. Vidu, R., et al., *Removal of Heavy Metals from Wastewaters: A Challenge from Current Treatment Methods to Nanotechnology Applications*. Toxics, 2020. **8**(4).
2. European, C., et al., *Study on the critical raw materials for the EU 2023 – Final report*. 2023: Publications Office of the European Union.
3. Prochaska, C. and G. Gallios, *Nano-Adsorbents for Cobalt Removal from Wastewater: A Bibliometric Analysis of Research Articles Indexed in the Scopus Database*. Processes, 2021. **9**(7): p. 1177.
4. Qasem, N., R. Mohammed, and D. Lawal, *Removal of heavy metal ions from wastewater: a comprehensive and critical review*. npj Clean Water, 2021. **4**.
5. Liosis, C., et al., *Heavy Metal Adsorption Using Magnetic Nanoparticles for Water Purification: A Critical Review*. Materials (Basel), 2021. **14**(24).
6. Allwin Mages Raj, A.F.P., et al., *Removal of Pb^{2+} , Cr^{6+} , and Hg^{2+} Ions from Aqueous Solutions Using Amino-Functionalized Magnetic Nanoparticles*. International Journal of Molecular Sciences, 2022. **23**(24): p. 16186.

Design of experiment methodology to improve dimethoate fluorescence detection

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Organophosphorus pesticides (OPs) pose a significant threat to humans, due to their toxicity, upon both high direct exposure and prolonged low-level exposure, which has been linked to cancer and non-Hodgkin lymphoma [1].

Dimethoate hydrolysed spontaneously in the environment leading to multiple products (figure 1) [2, 3] based on several parameters. Since our dye was sensitive to methylamine we tried to find the optimal hydrolysis conditions with the design of experiment methodology (DoE). We studied how NaOH concentration, temperature and time influence the hydrolysis. Moreover, since NaOH concentrated was degrading our dye, we also included in the DoE the pH at which we have to neutralize after the hydrolysis, to maximize the fluorescence.

Initially, the pesticide undergoes hydrolysis in a NaOH solution, yielding methylamine. Following neutralization, methylamine reacts with the dye in CH₃CN for 20 minutes. The optimization allows us to achieve an outstanding linear correlation ($R^2 = 0.999$) for dimethoate, spanning concentrations from 7.8 to 292 µg/L and LOD of 3.9 µg/L.

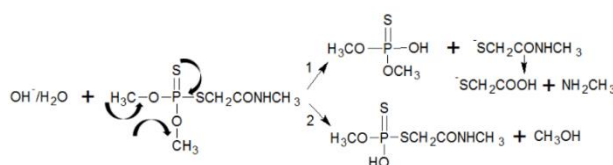


Figure 1. Two of the possible hydrolysis pathways of dimethoate²

References:

[1] M. Bagchi, S. Zafra, and D. Bagchi, *Toxicology of Organophosphate & Carbamate Compounds*, **2006**, 533-548.

[2] R. Farooq et al, *Journal of Shanghai University (English Edition)*, **2004**, 8, 221-226.

[3] L. Wu, J. Yao, P. Trebse, N. Zhang, & H. H Richnow, *Chemosphere*, **2014**, 111, 458–463.

Inverse Molecular Docking as a Powerful New Approach to Reveal Molecular Mechanisms of Polyphenolic Compounds from Turmeric and Rosemary

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Turmeric and rosemary represent evergreen medicinal plants with various beneficial health effects, including anticarcinogenic, antioxidative, anti-inflammatory, and antimicrobial effects. Curcumin represents the main polyphenolic compound responsible for the beneficial biological effects of turmeric, while the beneficial biological effects of rosemary can be attributed to diterpenes carnosic acid, carnosol, and rosmanol, as well as the phenolic acid ester rosmarinic acid. To discern intriguing and largely unexplored molecular mechanisms behind the pharmacological activities of polyphenolic compounds, a large-scale inverse molecular docking study was performed to identify potential protein targets of turmeric polyphenol curcumin, and major rosemary polyphenols rosmarinic acid, carnosic acid, carnosol, and rosmanol. Inverse molecular docking represents a unique computational approach to predict potential protein targets of natural products or small molecule drugs and, therefore, reveal their molecular mechanisms in various diseases. Inverse molecular docking was performed using our newly developed CANDOCK algorithm, which considers both protein and ligand flexibility. The individual polyphenolic compounds were docked to the predicted binding sites of all non-redundant holo-proteins from the Protein Data Bank, and their binding modes with prioritized target proteins were examined in detail. The predicted protein targets of curcumin from turmeric indeed revealed molecular mechanisms of its previously reported anticarcinogenic and anti-neuroinflammatory activities, while in the case of rosemary polyphenols, their potential anticoagulant and antiparasitic activity, as well as their inhibitory activity on HIV protease enzymes, was highlighted.

LCA for chemical recycling of waste PET bottles

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Currently, more and more attention is being paid to the recycling of PET bottles at the global level, whereby the "Life Cycle Assessment" method is used as a tool for assessing the impact of individual recycling phases, as well as for assessing the entire life cycle of PET bottles [2]. The most common type of plastic packaging is transparent polyethylene terephthalate (PET) bottles. The use of PET for the purpose of preparing plastic (food, industrial) packaging began to increase dramatically since 1970 [1]. Global market reports show that PET bottles account for 62% of all produced bottles, with an increasing amount returning to the recycling stream year after year. Thus, 28.4% of PET bottles were recycled in 2016 and 29.2% in 2017 [2].

In this work chemical recycling of transparent waste PET bottles was made with three different processes (neutral hydrolysis, neutral hydrolysis with purification method and alkaline hydrolysis). All of the processes were showing successful results (degradation efficiency > 99%), and were carried out on a scale – up. The final product of chemical recycling was secondary terephthalic acid in high purity (92% - 99%, depending on the process), which is considered a value – added end product that fetches high purchase prices on the market. The aim and goal of preparing the LCA analysis was to assess the environmental impact of the process and to determine the critical environmental indicators of the process. A "Gate-to-Gate" study was carried out (with GaBi software, method CML 2001-2016), which includes only processes from the production phase. The results of the study were compared with the LCA analysis production process of terephthalic acid of fossil origin. A comparison of the results of the LCA analysis of secondary terephthalic acid showed a lower impact on the environment compared to terephthalic acid of fossil origin in all cases.

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References:

1. Shen et al.: *Open-loop recycling: A LCA case study of PET bottle-to-fibre-recycling; Resource, Conversation and Recycling*, vol. 55, 2010.
2. Zhang et al.: *PET bottles recycling in China: An LCA coupled with LCC case study of blanket production made of waste PET bottles; Journal of Environmental Management*, vol. 260, 2020.
3. Xin et al.; *Journal of Environmental Management*, vol. 296, 2021.
4. Choudhary et al.: *Environment and economic impacts assessment of PET waste recycling with conventional and renewable sources of energy; Procedia CIRP*, vol. 80, 2019.
5. Marathe et al.: *Life Cycle Assessment (LCA) of PET Bottles; 2019*.

Multifunctional porous nanocomposites used in hybrid electrochemical filtration cell for efficient water purification

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Growth of population, emergence of new more persistent pollutants and lack of pure water resources pursue the research for improved water cleaning methods. Electrochemical filtration is a hybrid method combining the advantages of filtration and electrochemical cleaning techniques. In this method, the porous filtration material must be electrically conductive and thus serve also as an electrode.

For electrochemical filtration, we have prepared various porous electrodes as filtration material, consisting of fibrous templates and multifunctional nanomaterials. While fibrous templates provide porosity and stability, adding silver nanowires with good antimicrobial and conductive properties provides a high active surface area. To apply the needed external electrical current on the multifunctional filtration material, we have modeled a unique and adjustable filtration cell, which allows different operating parameters and component combinations for diverse or in-depth laboratory experiments. Finding the best component combination and operational parameters is crucial for efficient pollutant elimination.

The first trials show that electrochemical filtration can remove organic pollutants, decolorize dyes and disinfect model waters, with only one passing through the multifunctional filter material in the modelled electro-chemical filtration cell at a relatively low contact time and with low energy consumption. Due to the porous filtration material and dead-end filtration approach, the pollutants are forced into the vicinity of the multifunctional filtration material's surface, where antimicrobial effects and electrochemical processes occur. Electrochemical processes such as oxidation, reduction, indirect oxidation, charge repulsion, etc., occur on or near the electrode/filtration material simultaneously and the oxidizing/reducing agents are formed in situ in the cell.

The project's main aim is to optimize the porous nanocomposite used as a filter material and electrode for stable and improved antimicrobial as well as electrode performance and also to find the most appropriate operating parameters for efficient pollutant removal.

The results were created within the research project "Development of multifunctional nanocomposite fibrous electrodes for electro-oxidation filtration" (No. Z2-4483) and research program "Design of new properties of (nano) materials and applications" (No. P2-0424), The authors acknowledge the financial support from the Slovenian Research Agency ARIS.

Colloidal Coffee Waste Extracts Coatings on PLA films for Active Food Packaging

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Active packaging is an evolving technology aimed at preserving food quality. As per European Regulation, active materials refer to components deliberately added to packaging with the aim of prolonging shelf life or enhancing the condition of the food within. These materials are engineered to either release or absorb substances into or from the food or its surrounding environment ^[1].

While traditional methods like extrusion and blending are prevalent for incorporating active agents to the packaging, they often lead to the degradation of thermally unstable natural agents, reducing their surface availability. In contrast, coating films with active agents preserves the bulk material properties, improves surface interaction, increases contact area with food, and enables a controlled release, making it a more advantageous approach ^[2].

This study investigates the potential of coffee waste extracts, recognized for their antioxidant and antibacterial properties, as active agents for the surface functionalization of Poly(lactic acid) (PLA), a widely used biodegradable material in food packaging ^[3,4]. PLA films are coated using dip coating, with colloidal formulations of coffee extracts at varying concentrations. The inherently inert PLA surface is activated with plasma treatment prior to coating, to enhance the grafting of these bioactive compounds ^[5,6]. Schematic representation of the procedure is in figure 1.

The resultant coated films are analysed using various techniques. These included contact angle measurements to assess wettability, Attenuated Total Reflectance Fourier-Transform Infrared (ATR-FTIR) spectroscopy for surface composition analysis, Oxygen Transmission Rate (OTR) measurements to evaluate barrier properties improvement, and the ABTS assay to determine antioxidant activity. Antibacterial activity against Gram-positive *S. aureus* is also tested, along with Zeta potential measurements to monitor PLA film charge. The findings suggest that coffee waste extracts have the potential to improve the shelf life and quality of food products when used as coatings on PLA films. The colloidal coatings offer a significant advantage due to their availability at the surface, which is crucial for the interaction with food. This approach not only presents a sustainable solution for the food packaging industry but also emphasizes the benefits of utilizing colloidal coatings to enhance food preservation.

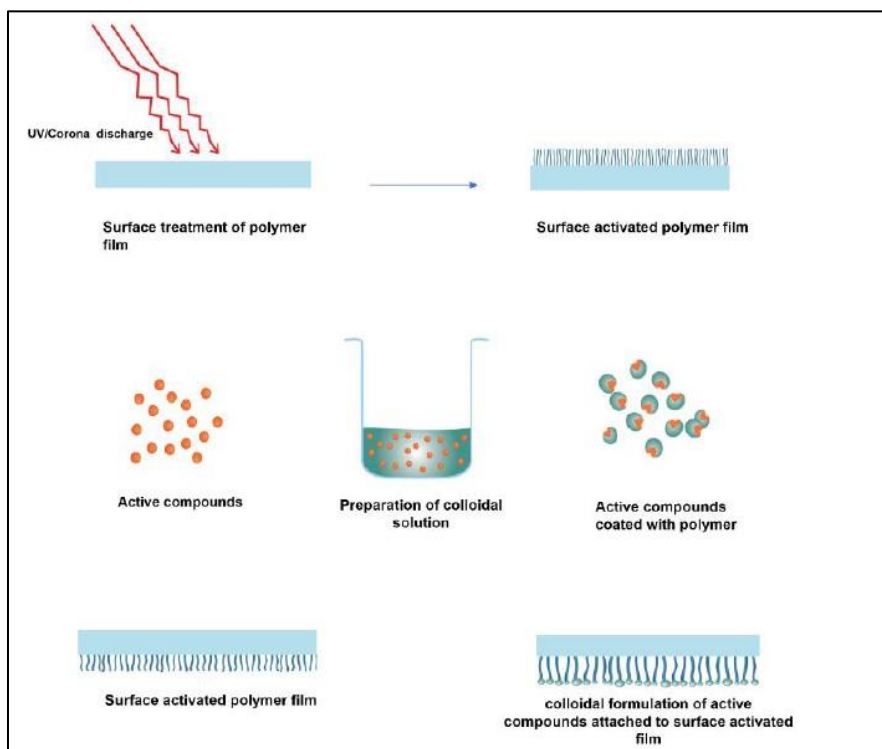


Figure 1 : Schematic representation of PLA films coated with colloidal coffee extracts.

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References

1. L. Barbosa-Pereira, G.P Aurrekoetxea, , I. Angulo, P. Paseiro-Losada, J.M Cruz, *Meat Science* (2014) 97, 249–254.
2. F. Debeaufort, Riondet, J. Brachais, C.-H. & N. Benbettaieb, *Coatings* (2022). **12**, 1–20
3. J. Simões, É. Maricato, F.M. Nunes, M.R. Domingues & M. A. Coimbra, *Carbohydrates Polymers* (2014) 101, 256–264.
4. A. S. P. Moreira, F. M. Nunes, M.R. Domingues, & M. A. Coimbra, *Food and Function* (2012) 3, 903–915.
5. D. Moradi, Y. Ramezan, S. Eskandari, H. Mirsaeedghazi, & M.J. Dakheli, *Food Packaging and Shelf Life* (2023) 35, 1-10.
6. A. Miletić, I. Ristić, M.B. Coltelli & B. Pilić, *Journal of Functional Biomaterials* (2020) 11, 1-16.

Recycling of cellulose materials

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Cellulose is a natural polymer composed of β -D-glucose units linked by β -1-4 glycosidic bonds, forming a linear chain. It is the most abundant organic polymer on Earth, predominantly found in the cell walls of plants, where it provides structural integrity and rigidity. The polymer chains aggregate into microfibrils, which further bundle into fibers, contributing to the mechanical strength and resilience of plant tissues. Cellulose's extensive hydrogen bonding network among hydroxyl groups results in a highly crystalline structure, conferring insolubility in water and resistance to many solvents and chemicals. In addition to its fundamental role in plant biology, cellulose has garnered significant interest in various scientific and industrial fields ^[1]. Its biodegradability, renewability, and abundance make it a sustainable resource for producing other biomaterials and valuable compounds like secondary fuel precursors ^[2].

Cellulosic waste materials, such as textiles, constitute a significant portion of municipal solid waste. Traditional methods of managing this waste, including landfilling and incineration, have numerous drawbacks, such as environmental burdens (soil, groundwater, and air pollution from incineration) and the loss of potentially valuable raw materials ^[3]. Hoping to contribute to solving this problem, the company IOS with its laboratory analyses and techniques, is working to successfully recycle cellulosic and cellulose-mixed raw materials, intermediates, and waste materials, resulting in value-added products such as glucose syrup and a solid residue as a by-product. Due to the interest in the potential for obtaining and evaluating the quality of glucose syrup, laboratory- and pilot-scale experiments on the decomposition of cellulosic materials using enzymatic hydrolysis were conducted.



Figure: Enzymatic hydrolysis of cellulose textile waste material (left) and pilot-scale batch reactor for cellulose material degradation (right)

References

- ^[1] O. J. Rojas, Ur., Cellulose Chemistry and Properties: Fibers, Nanocelluloses and Advanced Materials, let. 271. v Advances in Polymer Science, vol. 271. Cham: Springer International Publishing, 2016. doi: 10.1007/978-3-319-26015-0.
- ^[2] C. M. Cai, N. Nagane, R. Kumar, in C. E. Wyman, „Coupling metal halides with a co-solvent to produce furfural and 5-HMF at high yields directly from lignocellulosic biomass as an integrated biofuels strategy“, Green Chem, let. 16, št. 8, str. 3819–3829, 2014, doi: 10.1039/C4GC00747F.
- ^[3] N. C. Homem in M. T. P. Amorim, „Synthesis of cellulose acetate using as raw material textile wastes“, Mater. Today Proc., let. 31, str. S315–S317, 2020, doi: 10.1016/j.matpr.2020.01.494.

Production, isolation and purification of 5-HMF from cellulose waste material

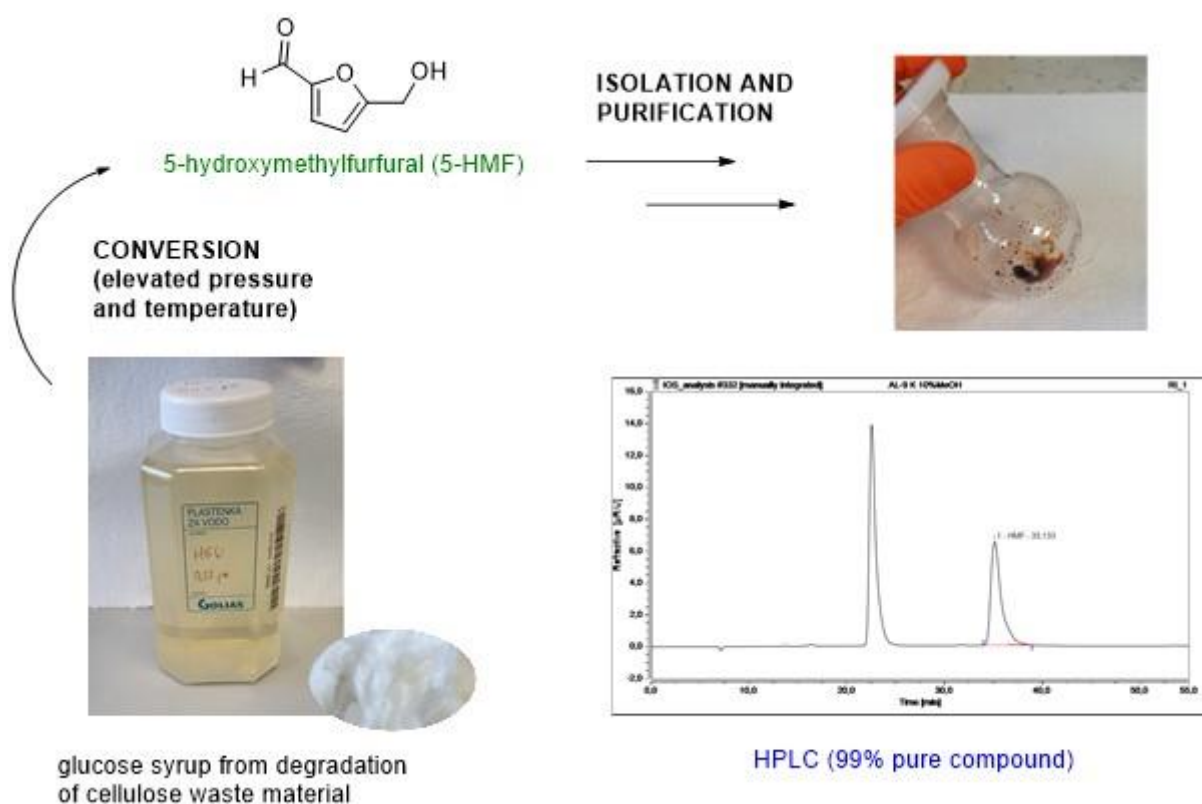
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5-hydroxymethylfurfural (5-HMF) is a promising platform chemical and a precursor for many value-added chemicals, such as bioplastics, liquid fuels and pharmaceuticals. In this study, we have successfully converted a glucose syrup, obtained by enzymatic degradation of cellulose waste material, to 5-HMF. The conversion reaction was performed using dehydration under elevated pressure and temperature [1]. Subsequent isolation of 5-HMF from reaction mixture was extensively studied, and 5-HMF was isolated as 99 % pure compound according to HPLC analysis. The structure of isolated 5-HMF was confirmed using high resolution NMR spectroscopy. These results represent a promising starting point for convenient isolation of 5-HMF from cellulose waste material and further optimization to suit the needs for the scale-up processes and industrial application.



References:

1. Jakob A, Likozar B, Grilc M. Aqueous conversion of monosaccharides to furans: were we wrong all along to use catalysts? *Green Chemistry* (2022) 24, 8523.

MerB (organomercurial-lyase) mediated quartz crystal microbalance (QCM) based Methylmercury detection

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Mercury is a highly toxic and mobile element that has had a pronounced and adverse effect on organisms. Accordingly, bacteria have evolved mer operons to meliorate the toxic action of different chemical forms of mercury. The bacterial mercury detoxification system contains two proteins, organomercurial lyase (MerB) and mercuric ion reductase (MerA). MerB specifically catalyses the protonolysis of the carbon-mercury bond of methylmercury (MeHg), resulting in the formation of a reduced carbon compound and inorganic ionic mercury (Hg²⁺).

Since MerB is a highly specific organomercurial lyase, we plan to use its Met-Hg-specific binding characteristics as a sensing/receptor component of the sensor. We intend to develop a Quartz crystal microbalance sensor (QCM) for detecting MeHg through the changes in the resonant frequency of a quartz crystal induced by the redox potential of Hg-bound-MerB after cleaving MeHg. On binding of MeHg onto MerB, we would determine the frequency and bandwidth of the crystal resonance.

To achieve that, we have prepared an expression system that will enable us to obtain enough highly active MerB enzymes. The expressed MerB enzyme with his-tag was purified and it showed High Hg-bound onto the MerB after cleaving from MeHg for preparing the Met-Hg-specific sensor. For the reporter system, We have prepared an SPE (Screen-printed gold electrode) and functionalized it with thiol followed by NTA-Ni²⁺ (Nitriloacetic acid with Nickel) for specific Histag MerB proteins binding and completed the initial characterisation.

MerB has been prepared as a specific bioreceptor for MeHg sensing, and Au@ NTA-Ni²⁺ electrodes were prepared as a platform for immobilization of Mer B and Mer A. We are planning to characterize furthermore on proteins immobilized in electrodes.

KEYWORDS: Methylmercury detection; Sensing: MerB (Organomercurial-lyase); Quartz crystal microbalance

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Gelatine nanoparticles loaded with the marine toxin APS7 increase the effectiveness of chemotherapeutic cisplatin on lung cancer cells

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Nicotine, which is responsible for smoking addiction, is not considered as carcinogen, but nicotine nevertheless has cancer-promoting effects through its action on the non-neuronal cholinergic system. Lung cancer cells express large amounts of nicotinic acetylcholine receptors (nAChRs), the ionotropic receptors on cell membranes that are the main target of nicotine. Binding of nicotine and other agonists to nAChRs leads to an increased Ca²⁺ influx and activates signaling pathways that trigger cancer cell proliferation, inhibit their apoptosis and increase cancer cell resistance to chemotherapeutics. This has led to the idea of using nAChR antagonists to attenuate the harmful effects of nicotine and other agonists. To avoid adverse effects of the antagonist on normal cells, it is important to deliver antagonist primarily to the cancer cells, which can be achieved by nanodelivery systems.

In our research, we have addressed the problem of chemotherapy resistance and off-target effects in the treatment of lung cancer. We have shown for the first time that the 3-alkylpyridinium salt APS7, a synthetic analog of a natural toxin from the marine sponge *Haliclona sarai*, acts as an antagonist of nAChRs, which reduces cancer stimulatory effects and increases efficacy of the chemotherapeutic agent cisplatin. In addition to free APS7, we prepared gelatin-based nanoparticles filled with APS7 (APS7-GNPs), which showed significant advantages compared to free APS7. They induced a greater reduction in lung cancer cell proliferation and selectively induced cytotoxicity to lung cancer cells, while they were not cytotoxic to non-tumorigenic lung cells. Our research demonstrates the potential of gelatin nanoparticles as a nanodelivery system for nAChR antagonists to improve chemotherapy efficacy and reduce off-target effects.

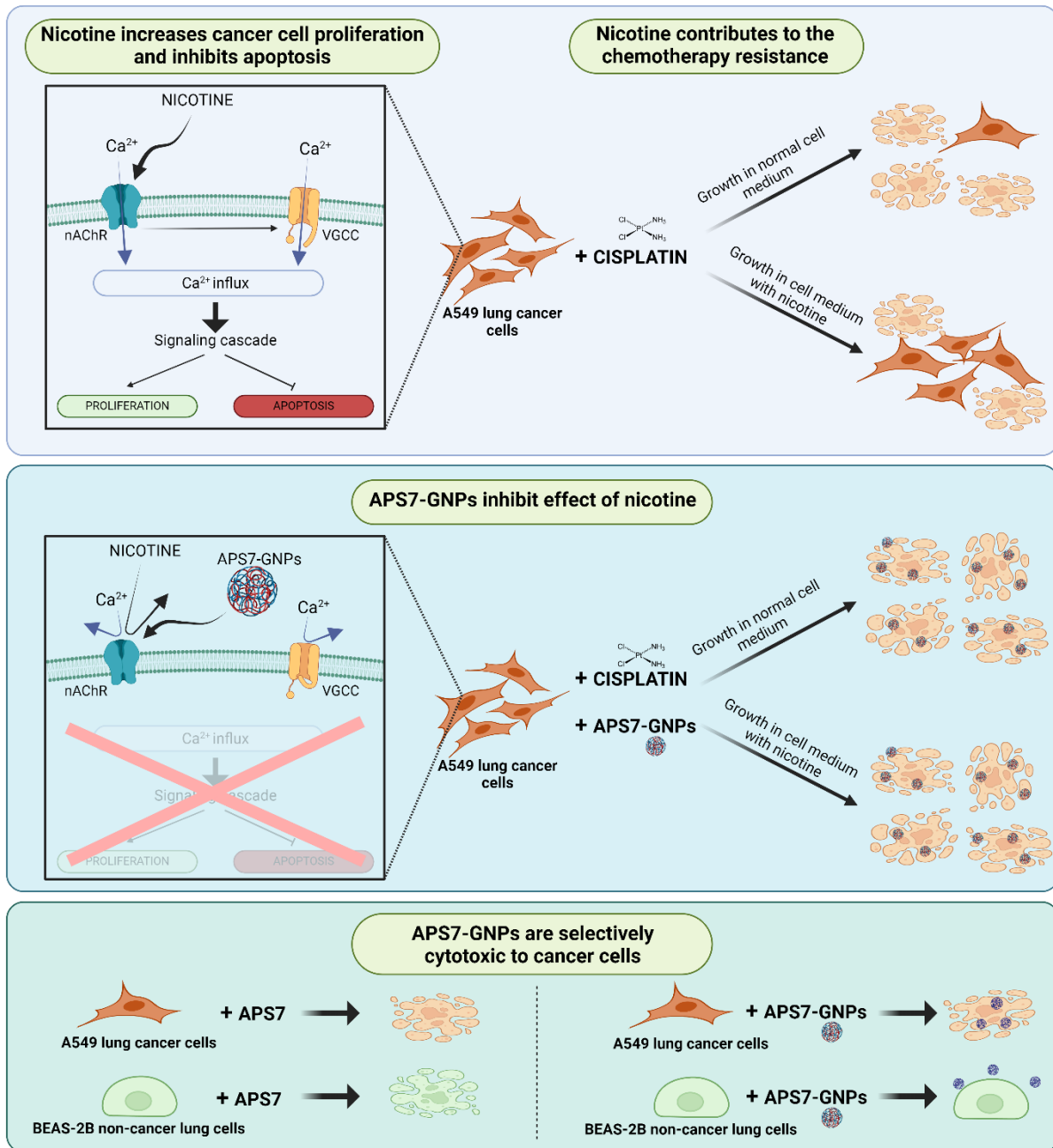


Figure 1. APS7 inhibits the pro-proliferative and anti-apoptotic effects of nicotine on lung cancer cells.

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CWA and TICs detection with multi-sensor platform GasSense

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This study introduces GasSENS, a compact and lightweight multi-sensor monitoring device developed through extensive experimental research and development to meet diverse gas detection needs. GasSENS measures up to eight gas analytes simultaneously, offering a versatile and reliable solution for precise environmental monitoring.

A key feature is its modular assembly, enabling easy sensor interchangeability with circular connectors, which simplifies customization for specific requirements. The device employs optical-chemical, electrochemical, and photoionization detection technologies to monitor a wide range of analytes, including chemical warfare agents (CWAs), and toxic industrial chemicals (TICs). Rigorous testing, including trials at the Military Laboratory Brno, demonstrated GasSENS's ability to detect TICs and CWAs below toxic levels (AEGLs).

GasSENS features an integrated air pump for consistent airflow, a particulate filter for enhanced measurement accuracy, and LED indicators for real-time status updates. Its rapid response time and automatic sensor detection enable timely, informed decisions. Ethernet communication using the MODBUS TCP/IP protocol ensures seamless integration with existing systems. Its compact and lightweight design allows for integration into unmanned aerial vehicles (UAVs) - drones, and other unmanned vehicles, expanding its application range.

GasSENS is part of the CBRN RSS system initiative, aimed at enhancing reconnaissance, surveillance, and incident management against CBRN agents. The system forms a transnational Intelligence, Surveillance and Reconnaissance (ISR) architecture for cooperative European-built CBRN capabilities, applicable in military operations, disaster relief, and high-visibility civilian events.

Antioxidant properties, chemical composition, and authenticity of rosemary and bay leaf essential oils in Slovenia

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Essential oils can be used as an antimicrobial biofilm in active packaging material, and their source and authenticity are essential to assuring relevant quality and safety. Our research was focused on two examples containing many functional bioactive compounds essential oils of rosemary (*Rosmarinus officinalis* L.) and bay leaf (*Laurus nobilis* L.).

Antioxidant properties, chemical composition, and authenticity of selected essential oils available on Slovenian market will be presented. The antioxidant activity was assessed using the DPPH method. The Folin-Ciocalteu method was employed to determine the concentrations of total phenolic compounds, and a positive correlation was found between the content of total phenolic compounds and the antioxidant activity of both rosemary and bay leaf essential oils. Using the TBARS assay, it was found that bay leaf essential oils were significantly more effective in inhibiting lipid peroxidation compared to rosemary essential oils.

The chemical composition of rosemary essential oils was analyzed by GC-MS, revealing a number of terpenoid compounds, among which 1,8-cineole and camphor were predominant, followed by monoterpene hydrocarbons such as α - and β -pinene, and oxygenated monoterpenes, including borneol and bornyl acetate. In the essential oil of bay leaf, 1,8-cineole was identified as the predominant compound, along with other compounds such as α -terpinyl acetate, sabinene, linalool, α -pinene, β -pinene, and methyl eugenol.

The carbon isotopic composition ($\delta^{13}\text{C}$) of the aromatic compounds in rosemary and bay leaf essential oils was determined by GC-C-IRMS. Analysis of one rosemary sample revealed a high limonene content and differences in $\delta^{13}\text{C}$ values, suggesting the addition of synthetic compounds or limonene-rich citrus essential oils. The observations for 1,8-cineole suggested the use of more readily available lavender essential oil to reduce costs. The isotopic analysis also indicated suspicions of adulteration in the three bay leaf samples, highlighting the need for further research of authenticity of commercial essential oils.

o-Phthaldialdehyde and 3-Mercaptopropyltriethoxysilane for Dopamine Detection: Experimental Results and Prospects

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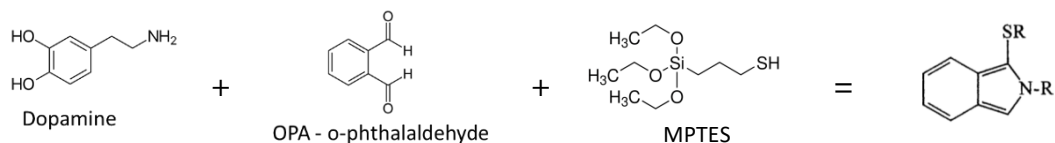
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Nanomaterials and sensors play an important role in modern technologies, including medical diagnostics and biochemical research^[1]. This work presents the possibility of using o-Phthaldialdehyde (OPA) in combination with 3-mercaptopropyltriethoxysilane (MPTES) to develop a dopamine-responsive sensor:



During the experiment, these materials were used at different pH and ratios to determine the optimal parameters for obtaining high fluorescence intensity of the reaction product ($\lambda_{ex}/\lambda_{em} = 340/434-458$ nm). The sensor response was measured using a fluorescence spectrometer. The data obtained demonstrate a linear relationship between the fluorescent response of OPA/MPTES and dopamine concentration in the range of 0.5-3.0 μM at pH 8, the detection limit was 32 nM.

The obtained results confirm the potential of OPA as a sensing component for the detection of biomolecules. Further research is aimed at covalently attaching OPA/MPTES to oxide-based substrates using Sol-Gel technology^[2] for develop sensor receptor of dopamine.

The authors acknowledge the financial support from the Slovenian Research and Innovation Agency (ARIS research programs Nos. P2-0424 and P2-0438).

References

1. P.-I. Gouma *Nanomaterials for Chemical Sensors and Biotechnology* (2010).
2. P. Nedeljko et al., *J Sol-Gel Sci Technol* (2016) 79(3).

Photo-induced synthesis of Prussian blue nanoparticles *in situ* on paper substrate for chemical sensing applications

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Recently, there has been a growing effort to incorporate biologically and ecologically friendly materials, such as paper and textiles, into various fields including sensor technology [1-3]. When combined with functional nanoparticles such materials offer numerous new possibilities due to their unique properties. However, a common issue with most nanoparticles is their toxicity and potential for bioaccumulation. Prussian blue (PB) is a mixed-valence polynuclear transition metal cyanide complex (iron(III) hexacyanoferrate(II)) and its nanoparticles are distinguished by their non-toxicity, greatly broadening their range of applications [4].

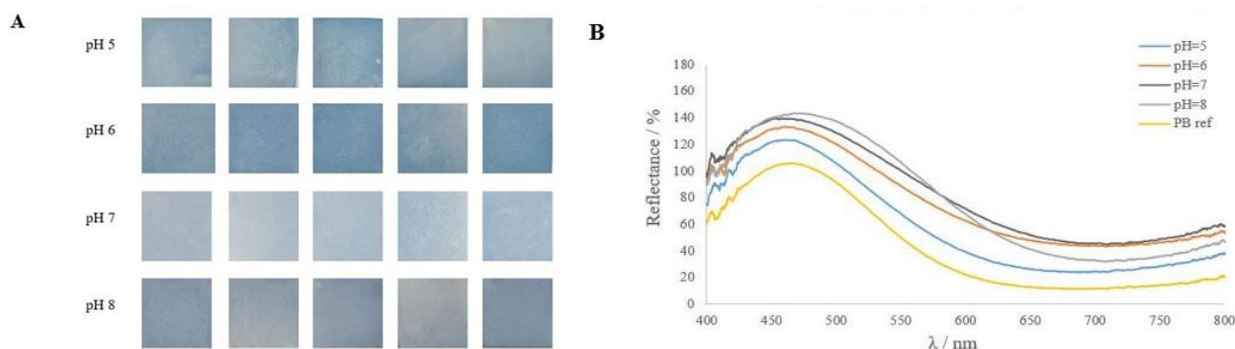


Figure 1. A-Paper strips immersed in buffer solutions in the pH range from 5 to 8, B- Reflectance spectrum of strips immersed in buffer solutions in the pH range from 5 to 8

In this study, the objective was to combine a biologically derived material (paper) with PB nanoparticles to create functional biocompatible material and explore its applicability as optical pH sensor. PB nanoparticles were successfully synthesized through *in situ* photoreduction by exposing the reagent loaded paper strips to UV radiation. Effects of exposure time, post-treatment conditions, concentration and ratios of reactants were studied and their effects on optical pH response, such as reversibility and stability, were examined. The colour change of paper strips exposed to different pH values can be detected visually (Figure 1-A), and by measuring reflectance spectra (Figure 1-B).

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References

1. S. Cinti, R. Cusenza, D. Moscone, F. Arduini, *Talanta* 187 (2018) 64
2. Y.-H. Zhu, X. Yang, D. Bao, X.-F. Bie, T. Sun, S. Wang, Y.-S. Jiang, X.-B. Zhang, J.-M. Yan, Q. Jiang, *Joule* 2 (2018) 746.
3. M Granica, Ł. Tymecki, *Analytica Chimica Acta* 1136 (2020) 133.
4. M. A. Busquets, J. Estelrich, *Drug Discov Today*. 25 (2020) 1443.

**Green all-cellulose biocomposites from renewable
biomass feedstocks produced in a water-based fabrication
system via the vacuum-filtration assisted impregnation pathway**

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All-cellulose composites (ACCs), a relatively new class of bio-composites fabricated solely from cellulosic raw materials, have emerged to fulfill the increasing demands and needs for more environmentally friendly and sustainable materials^{1–3}. In this research, sustainable ACCs were produced for the first time based on a complete dissolution of commercially available sulfite dissolving (D) pulps as a matrix at concentrations of 1.5 wt.% and 2.0 wt.% in an aquatic NaOH-urea solvent system. Subsequently, these cellulose matrix solutions were impregnated on/into pre-fabricated birch (B), abaca (A), and northern softwood (N) fiber sheets as reinforcements employing the vacuum filtration-assisted impregnation pathway. This study aimed to examine the effects of impregnated cellulose matrix concentrations and sorts of the used cellulose fiber reinforcements (B, A, N) on the morphological, crystalline, structural, and physio-mechanical properties of the ACCs. The most significant enhancements were observed in the tensile strength (+532%, from 9.24 MPa to 58.04 MPa) and strain at break of the B fiber-reinforced ACC B_{1.5} (+446%, from 1.36% to 4.62%), fabricated by the vacuum impregnation of the 1.5 wt.% cellulose matrix. Notably, substantial improvements were also noted in the elongation at break of the A and N fiber-reinforced ACCs A_{2.0} (+218%, from 32.76% to 54.93%) and N_{2.0} (+466%, from 2.59% to 14.65%), respectively, with a 2.0 wt.% cellulose matrix. This study highlights the diverse properties of ACCs, potentially driving further R&D for their upscaled production, particularly targeting their green packaging and environmental applications, such as fully bio-based mulching and warping materials.

References

1. Baghaei, B. & Skrifvars, M. All-Cellulose Composites: A Review of Recent Studies on Structure, Properties and Applications. *Molecules* **25**, 2836 (2020).
2. Uusi-Tarkka, E.-K. *et al.* All-Cellulose Composite Laminates Made from Wood-Based Textiles: Effects of Process Conditions and the Addition of TEMPO-Oxidized Nanocellulose. *Polymers* **14**, 3959 (2022).
3. Fujisawa, S., Fujisawa, S., Saito, T. & Isogai, A. All-Cellulose (Cellulose–Cellulose) Green Composites. in *Advanced Green Composites* (ed. Netravali, A.) 111–133 (Wiley, 2018). doi:10.1002/9781119323327.ch6.

Evaluating the Components of a Sample Holder System for Single Fiber Tensile Testing

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Cellulose fibers are known to display viscoelastic behavior during tensile testing, which influences the longitudinal modulus E [1, 2]. The sample holder system is the most commonly used type of mounting the cellulose fiber to the testing device and consisting of a polymeric sample holder, adhesive and a cellulosic fiber, it is difficult to determine if the obtained result represents the true properties of the fiber, or if it is affected by the sample holder and adhesive [3].

However, to ensure the obtained result corresponds to the true mechanical properties of cellulose fibers, the effect of the other two components in the sample holder system has to be looked into, evaluated and minimized.

Here we demonstrate that the influence of the sample holder and the adhesive on the E -modulus is not neglectable and the choice of the sample holder material and the type of the adhesive needs to be considered when planning to perform tensile testing on cellulose fibers.

In this work, the key components for tensile testing of cellulose fibers (sample holder and adhesive) are investigated, to determine their impact on the measured results. To eliminate one of the components, the cellulose fiber is replaced with a platinum wire, a purely linear-elastic material. Therefore, all non-linear responses from sample holder or adhesive can be identified. The component with the main influence on the results was the adhesive used to fixate the fiber on the sample holder and epoxy resin was found to be best suited. By taking these findings into the account, a series of tensile tests was performed on cellulose fibers, to demonstrate the validity of the system, but it is also applicable for tensile testing of any natural fiber.

References

1. Page, D. H., F. El-Hosseiny, and K. Winkler. 1971. "Behaviour of Single Wood Fibres Under Axial Tensile Strain." *Nature* 229 (5282): 252–253.
2. Jajcinovic, M., W. J. Fischer, A. Mautner, W. Bauer, and U. Hirn. 2018. "Influence of Relative Humidity on the Strength of Hardwood and Softwood Pulp Fibres and Fibre to Fibre Joints." *Cellulose* 25 (4): 2681–2690. Springer Netherlands.
3. Pickering, K. L., M. G. A. Efenfy, and T. M. Le. 2016. "A Review of Recent Developments in Natural Fibre Composites and Their Mechanical Performance." *Composites Part A: Applied Science & Manufacturing* 83:98–112.

Influence of iron oxide-based nanoparticles on the efficiency of polysaccharide coating as a potential modifier for the working electrode of an electrochemical sensor

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The increasing discharge of antibiotics into wastewater has become a major public concern. This situation emphasizes the urgent need for electrochemical sensors enhanced with precisely designed nanomaterials to detect antibiotics in contaminated environments. Various nanomaterials have been investigated for their increased sensitivity and unique properties. Usually, materials such as graphene, carbon nanotubes, metals and conductive polymers have mainly been used in the modification of electrode surfaces. However, these materials are limited by high synthesis costs, difficulties in removing metal catalysts, hydrophobicity, agglomeration problems and induced defects, which limit their efficiency in the development of highly effective modified electrochemical sensors ^[1,2]. In contrast, magnetic iron oxide nanoparticles (MNPs) offer a promising alternative due to their controlled synthesis conditions and potential for functionalization with biopolymers. MNPs offer advantages such as a large surface area, excellent electron conductivity and more electroactive interaction sites. Despite these advantages, there are still significant research gaps, particularly in the development of MNPs functionalized with polysaccharides with specific properties for use as modifiers in electrochemical sensors. This study focused on the preparation of magnetic iron oxide nanoparticles (MNPs) functionalized with carboxymethyl dextran (CMD), a polysaccharide with specific functional groups. The aim was to use this modified material as a potential electrochemical sensor to improve sensing capabilities. Two different modification methods were tested to evaluate the effects of magnetic nanoparticles on the efficiency of the CMD coating. In the first method, MNPs were synthesized by hydrothermal synthesis using iron sulfate salts, stabilized with citric acid, and coated with an approximately 2 nm thick porous silica (SiO₂, abbreviated as S) layer to increase the specific surface area. The MNPs were then functionalized with aminopropyl triethoxysilane (APS; abbreviated as A) to introduce -NH₂ groups, which give a positive charge under moderately acidic conditions. CMD was electrostatically attached to these MNPs@S@A particles, resulting in MNPs@S@A-CMD. In the second procedure, the MNPs were directly silanized with APS and subsequently functionalized with CMD, resulting in MNPs@A-CMD. The resulting nanocomposites were characterized using transmission electron microscopy (TEM) to assess the morphology, size and effectiveness of the silica coating. Further characterization included infrared spectroscopy, electrokinetic measurements of zeta potential, X-ray photoelectron spectroscopy (XPS), thermogravimetric analysis and evaluation of magnetic properties. The results showed that the formation of all desired layers on the MNPs was successful in both methods, with the final CMD layer having functional groups (hydroxyl and carboxyl) that can enhance the adsorption

of antibiotics and consequently electrochemical response. This result suggests that CMD-functionalized MNPs have significant potential as effective modifiers for electrochemical sensors targeting antibiotics.

References

1. R. Jain, N. Jadon and A. Pawaiya, *TrAC - Trends Anal. Chem.*, 2017, **97**, 363–373.
2. E. Asadian, M. Ghalkhani and S. Shahrokhian, *Sensors Actuators, B Chem.*, 2019, **293**, 183–209

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Combating Hospital-Acquired Infections with Antiviral Polysaccharide Coatings for Personal Protective Equipment: A Physicochemical Analysis of Liquid Media

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The 2019 Coronavirus pandemic outbreak highlighted the critical need for strategic antiviral coatings on textile personal protective equipment (PPE). Hospital environments, which, due to their function, have a high level of risk for the cross-spread of pathogenic microorganisms, commonly experience costly and deadly hospital-acquired infections ^[1]. We have characterized key physicochemical properties of differently concentrated aqueous solutions of polysaccharides (1-5 mg/mL) with promising antiviral activity that are either anionic or cationic (poly)electrolytes, i.e., dextran sulfate, λ -carrageenan, chondroitin sulfate A, fucoidan, quaternary chitosan, carboxymethyl chitosan and carboxymethyl dextran. We utilized techniques for determining molecular composition, zeta potential and hydrodynamic diameter, as well as bioactivity assessments (i.e., antioxidant and antimicrobial activity), and analyses of physical properties (i.e., thermal stability, viscosity, surface tension). Attenuated total reflectance-Fourier transform infrared spectroscopy (ATR-FTIR) and zeta potential (ZP) determinations confirmed that the polysaccharides contain characteristic active functional groups (e.g., carboxyl, sulfate, sulfonic acid, hydroxyl, primary and quaternary amino, etc. groups), and moderate to high values of ZP in the pH range between 3 and 9. High ZPs ($\geq \pm 25$ mV), suggesting dispersion stability, were expressed by dextran sulfate, quaternary chitosan, fucoidan and λ -carrageenan solutions. Particle size distribution, hydrodynamic diameter and turbidimetry assessments revealed that the solutions contain heterogeneous colloidal particles. Polysaccharide solutions did not show significant antioxidant (conc. 0.01-1 %) or antibacterial activity (at conc. ≤ 0.5 %; excluding quaternary chitosan). Similarly, only quaternary chitosan solution exhibited an antiviral effect with a 2.49 log reduction of plaques ($\phi 6$ infected *Pseudomonas syringae* cells).

References

1. G. Suleyman et al., *Current Infectious Disease Reports* (2018) vol. 20, p. 12.