

Przesieka, May 17-19, 2024 INTERDISCIPLINARY DOCTORAL SYMPOSIUM

BOOK OF ABSTRACTS





Wrocław University of Science and Technology



RAJD DOKTORANTA 2024

INTERDISCIPLINARY DOCTORAL SYMPOSIUM

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Przesieka, 17-19 May 2024



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Lithium-oxygen batteries - exceptional solution to ordinary problem

Denis Kopiec, Krzysztof Kierzek

Department of Process Engineering and Technology of Polymer and Carbon Materials, Wrocław University of Science and Technology

Denis Kopiec: denis.kopiec@pwr.edu.pl

One of the pressing challenges faced by today's world is the growing demand for energy storage capacity. This evergrowing need is linked to the expansion of electric vehicles sector and the pursuit of efficient technology for the industrial energy storage sector, for example in storage for the energy from renewable sources. Lithium-oxygen (Li-O₂) batteries are proposed as a promising response to these challenges, owing to their exceptionally high specific energy (~3500 Wh kg⁻¹) and lightweight characteristics. These advantages result from the semi-open system in which Li-O₂ batteries operate and the oxygen reduction and evolution reactions (ORR/OER) occurring during discharge and charge cycles. However, these factors put specific demands on cathode materials, including a large specific surface area, suitable porous structure, high electrical conductivity, and catalytic activity in ORR/OER. This work will briefly outline the operational principles of Li-O₂ cells and the critical requirements for cathode materials. Moreover, it will explore the significance of advancing new energy storage technologies and discuss the primary benefits of lithium-oxygen cells.

Keywords: lithium-oxygen batteries, energy storage, cathode materials, carbon nanomaterials

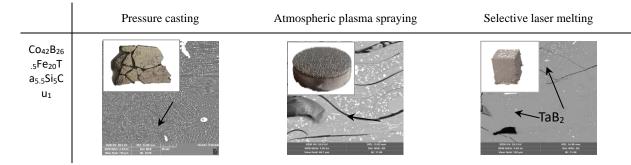
Processing ability of alloy with high-glass forming ability Co₄₂B_{26.5}Fe₂₀Ta_{5.5}Si₅Cu₁

Anna Kuś¹, Wirginia Pilraczyk², Viktória Rajťúková³, Radovan Hudák³, Paweł Sokołowski¹, Thomas Mehner⁴, Thomas Lampke⁴, Mathieu Tartarin⁵, Aleksandra Małachowska¹

¹ Wrocław University of Science and Technology, Wybrzeże Wyspańskiego 27, 50 370 Wrocław, Poland
 ² Silesian University of Technology, Akademicka 2A, 44-100 Gliwice, Poland
 ³ Technical University in Kosice, Faculty of Mechanical Engineering,
 Department of Biomedical Engineering and Measurement, Letná 1/9, 040 01 Košice, Slovakia
 ⁴ Materials and Surface Engineering Group, Institute of Materials Science and Engineering,
 Chemnitz University of Technology, 09107 Chemnitz, Germany
 ⁵ University of Limoges, 33 Rue François Mitterrand, 87000 Limoges, France

isity of Elinoges, 55 Rue François Mitterfand, 67000 Elinoges, Fr

Anna Kuś: anna.kus@pwr.edu.pl



Alloys with high glass forming ability are currently in the interest of researchers around the world. The high glassforming ability can provide manufacturing 100% amorphous structure of the produced elements. The most important requirement for obtaining such a structure is the cooling rate (R_c) for rapid solidification processes (RSP). This research focused on the three RSPs, namely, pressure casting, plasma spraying, and selective laser melting (SLM). All of the mentioned processes can meet the requirements of high enough R_c if the process parameters are properly arranged. Additionally, concerned alloy must have a high enough glass forming ability (GFA) which can be determined experimentally [1,2].

The alloy of interest in this work is $Co_{42}B_{26.5}Fe_{20}Ta_{5.5}Si_5Cu_1$ and was obtained by alloying pure chemical elements. The obtained master alloy was used for pressure casting of plates in copper dies and for gas atomization into powder for SLM and plasma spraying. The parameters for each process were determined by a literature study and several experimental tests. To determine the processing ability of $Co_{42}B_{26.5}Fe_{20}Ta_{5.5}Si_5Cu_1$ the metallurgic cross-section was done and observed with optical microscope and electron scanning microscope (SEM). The presence of an amorphous phase was checked by X-ray diffraction. To determine the influence of the processes on mechanical properties, the nanoindentation test was conducted.

Samples of all technologies have been developed successfully, including SLM printing, which is one of the first uses of this technology for Co-based alloys with high glass-forming ability. Microscopic observation of the casted plates shows the problem of cracking while cooling. Similar observations were made in the SLM printing. This phenomenon is connected to remarkably high temperature gradients while cooling the samples, leading to thermal stress that exceeds the mechanical strength of the alloy and, in consequence, leads to cracking. In plasma-sprayed samples, the cracking process was not observed; however, delamination of some splats was observed. Furthermore, microscopical observations of each sample show the problem of crystallization, leading to the formation of composites built from amorphous matrix with crystal precipitations. XRD analysis shows that the crystal phases were, in fact, mainly TaB₂ and some Co₅Si₂B. TaB₂ in SEM observations were seen as brighter spots, and the nanoindentation test confirmed the very high hardness of those phases, which is consistent with the literature reports. The hardness results were correlated with the degree of crystallization of the samples. A casted plate that exhibits the highest crystallization (observed by SEM) of the mentioned hard phase had the highest harness on the level of 17 GPa, while samples manufactured by SLM, and plasma spraying had similar values of hardness around 14.5 GPa.

In summary, the alloy $Co_{42}B_{26.5}Fe_{20}Ta_{5.5}Si_5Cu_1$ can be processed by pressure casting, plasma spraying, and selective laser melting. However, the GFA of this alloy is not high enough to provide a fully amorphous structure, which limits the size of the obtained sample by casting and leads to defects in the plasma spraying process and SLM such as delamination and cracking, respectively.

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Muscle Fructose 1,6-bisphosphatase (Fbp2) as an regulator of mitochondrial dynamics in cancer and healthy cell lines

Łukasz Pietras, Agnieszka Gizak

Department of Molecular Physiology and Neurobiology, University of Wrocław

Łukasz Pietras: lukasz.pietras2@uwr.edu.pl

Muscle fructose 1,6-bisphosphatase (Fbp2) is an isoform of an glycogenesis enzyme, which catalyzes dephosphorylation of fructose-1,6-bisphosphate to fructose-6-phosphate. This process opposites glycolysis, and its catalytic activity promotes glycogen formation from glucose.

Cancer cells produce an energy in form of ATP from lactate fermentation, which includes glycolysis with no mitochondrial respiration. Mitochondrial respiration is often still major source of ATP, however ability to create ATP without oxygen enhanced cancer cells proliferation. Marginalization of mitochondrial respiration requires changes in mitochondrial metabolism. Key mitochondrial metabolism regulator is mitochondrial dynamics-processes which contributes mitochondrial shape, volume and localization. Differences in mitochondrial dynamics in healthy and cancer cells are intensively studied by scientists around the world. Results are far from conclusions. One major problem is unclear mechanisms of mitochondrial fusion and fission, mitochondrial trafficking and mitochondrial autophagy [1].

During authors master degree work, author has discovered that Fbp2 regulates mitochondrial transport velocity. Fbp2 functions in cells as an oligomers. Fbp2 plays an important role in many fields, despite its catalytic role. That nocatalytic activity relies on protein-protein interaction and subcellular localization. Fbp2 protein interactors and localization results from oligomeric form: dimeric or tetrameric. Fbp2 dimers co-localize with mitochondria, and interacts with mitochondrial protein. In master degree work, chemically induced tetramerization which delocalizes Fbp2 from mitochondria, slower mitochondrial transport velocity. During PhD studies, author discovers also, that dimer of Fbp2 promotes mitochondrial activity, decrease mitochondrial autophagy level and promotes mitochondrial elongation in healthy cells. It was correlated with healthy cells better condition [2]. However in cancer cells, that effects has not appeared. It was discovered that in majority of cancers Fbp2 is completely or partially silenced, due its anti-oncogenic role. Lower amount of Fbp2 is correlated with worse prognosis, and its elevates a risk for malignation of cancer (higher metastasis risk). Authors results suggest that in studied cells Fbp2 has lower potential for mitochondrial dynamics regulation, but its plays still some role. Complete silencing of Fbp2 expression has improved mitochondrial activity in cancer cells (inversely to healthy cells), but it has slowed down their proliferation. Later studies suggest, that Fbp2 silencing in studied cells provides to appearance of metastatic phenotype. That result also confirms that Fbp2 is an anti-oncogenic protein, which can be treated as an target for anti-cancer treatment. However, authors research puts some questions in precise role of Fbp2 in mitochondria functioning. Since now, it is clear that Fbp2 work differently in cancer and healthy cells. But why and in which mechanism is still not known.

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Keywords: mitochondria, cell metabolism, cancer, cell lines, organelles, Fbp2

Exploring Aging Through Metabolomics

Natalia Pudełko-Malik¹, Dominika Drulis-Fajdasz², Dariusz Rakus², Piotr Młynarz¹

¹ Department of Biochemistry, Molecular Biology and Biotechnology, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370, Wrocław, Poland ² Department of Molecular Physiology and Neurobiology, University of Wrocław,

Sienkiewicza 21, Wrocław, 50-335, Poland

Natalia Pudełko-Malik: natalia.pudelko-malik@pwr.edu.pl

Understanding the complexities of ageing requires a comprehensive investigation into the physiological changes that occur over time. Metabolomics, as an analytical profiling technique, offers a powerful tool to explore into the intricate metabolic alterations associated with ageing [1]. This abstract explores the pivotal role of metabolomics studies in unravelling the mysteries of ageing. Through the analysis of small molecules, known as metabolites, in biological samples, metabolomics provides valuable insights into the dynamic changes occurring within ageing organisms.

Nuclear Magnetic Resonance Spectroscopy (NMR), a widely utilized technique in metabolomics research, particularly in the study of brain metabolism, enables researchers to delve deep into the biochemical intricacies of ageing. By examining metabolic pathways across different developmental stages, metabolomic approaches offer a nuanced understanding of age-related changes in phenotypic, physiological, and functional states [2].

This abstract highlight the importance of employing metabolomics methodologies to elucidate age-related biomarkers and unravel the complex interplay of biochemical pathways underlying the ageing process. Through metabolomics studies, researchers can gain crucial insights into the molecular mechanisms driving ageing, paving the way for the development of targeted interventions and therapeutic strategies to promote healthy ageing and improve quality of life [3].

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Keywords: metabolomic, nuclear magnetic resonance spectroscopy (NMR), ageing

Experimental study of the aggregation ability of selected peptides produced by the human microbiome with consideration of cross-interactions

Oliwia Polańska¹, Monika Szefczyk², Małgorzata Kotulska¹

¹ Department of Biomedical Engineering, Wroclaw University of Science and Technology ² Department of Bioorganic Chemistry, Wroclaw University of Science and Technology

Oliwia Polańska: oliwia.polanska@pwr.edu.pl

Neurodegenerative diseases (NDDs) are characterized by progressive damage to nerve cells in various brain areas, leading to impaired cognitive functions. Alzheimer's Disease (AD) is an example of NDDs. It is characterized by the presence of amyloids – protein aggregates such as amyloid beta (A β), which accumulate in the brain, disrupting its function [1]. Amyloids form during the aggregation process and create fibers that are resistant to many factors with a characteristic β -cross structure [2].

Amyloid peptides can interact with other peptides or proteins, resulting in e.g., accelerated aggregation processes and the formation of heteroaggregates – assemblies composed of different peptides or/and proteins. Literature has described, among others, the co-occurrence of A β with α -synuclein (a protein associated with Parkinson's disease) and A β with amylin (type II diabetes) [3].

The amyloids and their interactions can be studied using experimental techniques such as:

- thioflavin T dye binding assay for studying aggregation kinetics;
- infrared spectroscopy and circular dichroism spectroscopy for determining secondary structure;
- high-resolution microscopy, such as atomic force microscopy (AFM) or electron microscopy (EM), for examining the morphology of the aggregates formed [4].

Besides disease-related amyloids, functional amyloids are also distinguished. They are found, e.g., in certain bacteria belonging to the human microbiome, with their largest clusters located in the intestines. Some peptides produced by these bacteria can aggregate, allowing them to perform various functions, such as stabilizing the biofilm. This provides the bacteria with resistance to adverse environmental conditions [3, 5].

The gut microbiota can communicate with the brain, among other ways, through the so-called gut-brain axis [5]. In this way, bacterial peptides may promote amyloid formation, contributing to the development of various NDDs. Recent studies have confirmed a link between changes in the gut microflora and neurological disorders [2, 6]. An example of a bacterium associated with AD is *Helicobacter pylori* [6]. This bacterium produces an aggregable protein Hpn (histidine-rich protein) [7]. Investigating the influence of Hpn presence on A β aggregation is the goal of this research and may contribute to a better understanding of the pathogenesis and spread of AD. Confirming the hypothesis that the presence of Hpn accelerates the A β aggregation process will indicate that *H. pylori* infection is not indifferent to human health and may contribute to the development of AD.

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Keywords: amyloids, peptide aggregation, cross-interactions, neurodegenerative diseases, human microbiome

Characteristics of waste biomass and biochars obtained from it assessment of potential applications

Natalia Niedzbała¹, Piotr Rutkowski², Izabela Michalak¹

 ¹ Department of Advanced Material Technologies, Faculty of Chemistry, Wrocław University of Science and Technology, Poland
 ² Department of Process Engineering and Technology of Polymer and Carbon Materials, Faculty of Chemistry, Wrocław University of Science and Technology, Poland

Natalia Niedzbała: natalia.niedzbala@pwr.edu.pl

Continuous population growth causes increased consumption and the need to increase the surface area of agricultural land. In addition, continuous climate changes, which causes the intensification of negative phenomena such as warming, floods, chemicalization, drastically worsens the condition of the soil and environment, force the search for innovative solutions. These negative consequences of environmental change and population growth can be partially minimized by using biochar (especially produced from waste biomass) in agriculture and environmental protection.

The aim of this study was to characterize waste biomass, i.e., spend coffee ground, banana peels, marine algae (Cladophora glomerata), and biochar obtained from this biomass for subsequent applications. The pyrolysis process was used to obtain valuable bioproducts (biochars) from waste biomass at a process temperature of 450 °C, heating rate 10 °C/min, residence time 1 h. Proximate analysis (moisture, volatile matter, ash content), pH, electrical conductivity (EC), elemental analysis (C, H, N, S), multielement analysis (using ICP-OES and XRF technique), FTIR analysis were used to characterize waste biomass and biochars. Additionally, the efficiency of the pyrolysis process and the pH_{PZC} values were determined for biochars. The pyrolysis yield for the algal biochar was 60.7 ±1.4%, for banana biochar was $39.2 \pm 4.0\%$, and for coffee biochar was $25.8 \pm 1.4\%$ (N = 2). After thermal conversion of waste biomass, there was a decrease in volatile matter and an increase in ash content for all biochars, while the moisture content decreased except for banana biochar compared to raw materials. Investigating the pH, electrical conductivity of waste biomass and biochars, and tpHhe pH_{PZC} of biochars will be crucial for further research into their potential applications. Higher pH values (measured in aqueous solutions) were obtained for biochars (for algae 8.88 ±0.02, banana 9.85 ± 0.01 , coffee 9.89 ± 0.14) compared to waste biomass (for algae 6.73 ± 0.01 , banana 5.14 ± 0.01 , coffee 5.54 ± 0.08). However, the conductivity value depended on the raw material used. For banana biochar (22.9 ± 3.1 mS/cm) there was an increase in EC value compared to banana peels (12.2 ± 0.2 mS/cm), for coffee biochar $(0.463 \pm 0.004 \text{ mS/cm})$ there was a decrease in EC value compared to the raw material $(0.802\pm 0.194 \text{ mS/cm})$, and for algal biomass (15.0 \pm 0.2 mS/cm) and its biochar (15.1 \pm 0.3 mS/cm) there was no change in value. The pH_{PZC} values for biochars were 7.56 ± 0.03 for coffee, 7.73 ± 0.01 for algae, and 9.41 ± 0.02 for banana. After conducting elemental and multielement analysis of raw materials and biochars, it can be concluded that both raw materials and biochars had a high content of macroelements such as calcium, potassium, magnesium, sodium, phosphorus, sulfur. The high content of macroelements, especially potassium increases the EC values of both biomass and biochar. In addition, higher element contents were obtained for biochars compared to raw materials except for hydrogen, phosphorus, sulfur for banana and coffee. The analysis of functional groups on the surface of biomass using FTIR technique allowed the conclusion that both the raw materials and biochars contain groups such as: O–H, aliphatic C–H, C=C, C–N, aromatic C–H, C–O, and only for algae there is vibration Si–O–Si.

After the characterization of waste biomass and biochars, it can be concluded that biochars could be used as a soil additive due to the high content of macroelements and high pH (addition to acidified soil to correct the pH). In addition, biochar can be used to remove pollutants from wastewater due to the presence of functional groups that can participate in the binding of heavy metal ions.

Keywords: waste biomass, pyrolysis, biochar, characterization of biomass/bioproducts, environmental protection

Modification of polyesters based on 2,5-furandicaroboxylic acid

Konrad Walkowiak

Department of Mechanical Engineering and Mechatronics, West Pomeranian University of Technology in Szczecin

Konrad Walkowiak: wk42388@zut.edu.pl

If current growth rates are maintained, worldwide plastics production will reach 1124 million metric tons annually 2050 [1]. Currently, most polymeric materials are based on fossil-based monomers, which consume plenty of petrochemical resources when combined with a decline in fossil fuels and the nondegradability of fossil-based polymers, it caused a turn to develop new, sustainable sources. Apart from oil and coal, biomass is the most appealing alternative feedstock since it is the only generally available carbon source. Nevertheless, most of the currently produced biobased polymers, like polylactic acid, polybutylene succinate, or polyglumatic acid, have an aliphatic structure, while petroleum-based engineering plastics have mostly aromatic structure. Therefore, the development of bio-based materials with aromatic structure plays a key role in substituting traditional petroleum-based polymers. The most discussed bio-based aromatic monomers are (purified) terephthalic acid (PTA), 2,5-furanodicarboxylic acid (FDCA), and vanillin (Fig. 1). FDCA was selected as one of the 12 most promising bio-based platform compounds by the U.S. Department of Energy and is the only bio-based aromatic chemical in that list.

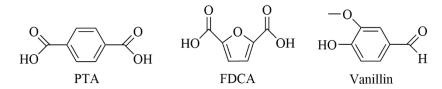


Fig. 1. Chemical structure of bio-based aromatic monomers

The most representative and well-analyzed FDCA-based polyester is poly(ethylene furandicarboxylate) (PEF), which is an alternative to commercially available PET. The reports considering PEF show that it has more attractive thermal and mechanical properties than PET [2]. The PEF also has superior barrier properties, its oxygen permeability is 10 times lower, and CO₂ permeability is 19 times lower than PET. Higher thermal, mechanical, and barrier properties of PEF when compared to PET result from the rigid structure of the furan ring and suppressed furan ring flipping. Special emphasis is placed on efforts to tailor polymer compositions and architectures through polymer chemistry. Isosorbide is an important bio-based monomer for high-performance materials. Isosorbide has a rigid structure and is bi-heterocyclic diol derived from glucose. The polymers based on isosorbide possess excellent properties such as strong resistance to UV radiation, heat, chemical degradation, and tensile properties. Moreover, polymers containing isosorbide have found application as biomedical engineering materials due to their biodegradability and biocompatibility [3] and also for the production of packing and electronic displays. In 2014, 35% of produced isosorbide was used to produce (poly(ethylene-co-isosorbide) terephthalate (PEIT). However, only a few studies have been carried out on bio-based copolyesters based on isosorbide and FDCA concerning an increase in glass transition temperature. The furan-based polyester can also be modified by using diol, the introduction of long-chain flexible diols can improve the toughness of FDCA-based polyesters. The evolution of bio-based aliphatic diacids and diols caused all common petroleum-based aliphatic copolymers to have their bio-based alternative. Linear aliphatic polyesters based on raw materials of plant origin are semicrystalline, and most studies focus on modifying their thermal and mechanical properties and degradability by adjusting the number of methylene groups. The increase of methylene groups causes a decrease in the value of glass transition. Nevertheless, an increase in methylene groups results in a higher regularity of molecular chains and a lower density of ester groups, reducing the rigidity of molecular groups and facilitating crystallization. Thus, incorporating linear aliphatic chain units alters the thermal properties, mechanical properties, and degradation of polyesters.

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Keywords: polyesters, copolymers, melt polycondensation, supramolecular structure, FDCA

Dam failure mechanisms - results of scale laboratory tests

Krzysztof Zamiar, Mikołaj Urbaniak, Stanisław Kostecki

Department of Geotechnics, Hydrotechnics, Underground and Water Engineering, Faculty of Civil Engineering, Wrocław University of Science and Technology

Krzysztof Zamiar: krzysztof.zamiar@pwr.edu.pl

This work presents model studies of the erosion of a homogeneous geotechnical embankment made of non-cohesive soils carried out in the field laboratory of the Wrocław University of Science and Technology. Understanding the destruction process of such structures, including earth dams and flood embankments, is crucial to determining the amount and rate of released water. This is necessary to assess the consequences of catastrophe, analyse the risk, and develop appropriate crisis management procedures. The dam tested is 0.50 m high and closes a reservoir with a capacity of 14.4 m³. The width of the test site did not restrict the width of the breach. The scenario analysed assumes that water overflows the crest of the embankment, as it is the most common cause of embankment failure based on databases cataloguing dam disasters [1]. At the same time, the amount of water accumulated in the reservoir in this scenario is the largest possible, suggesting that such a disaster could have the most severe consequences. Based on the results of three experiments, four repeatable phases of erosion evolution were identified and described: (I) the initial phase, (II) the vertical erosion phase, (III) the lateral erosion phase, divided into two cycles, and (IV) the reservoir emptying phase without further propagation of the breach. The final width of the breach created each time was between 2.2 and 2.5 H (where H is the height of the embankment). Although the third test was much faster and the peak discharge had a higher value this did not affect the final width of the breach.

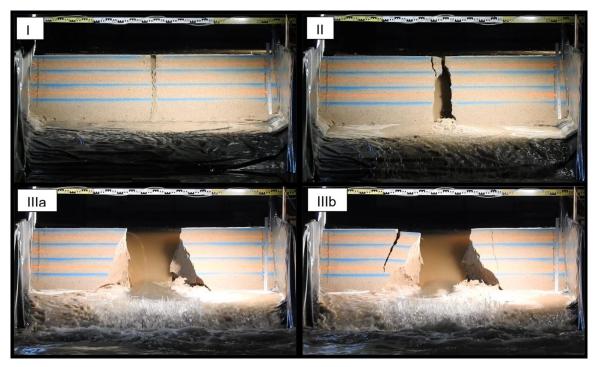


Fig. 1. Analysed embankment during: (I) the initial phase, (II) the vertical erosion phase, (IIIa) the lateral erosion phase cycle a, (IIIb) the lateral erosion phase cycle b

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Keywords: dam safety, flood risk management, overtopping, breach parameters, breach mechanism

Biological properties of halogenated flavonoids and biophysical characterization of their liposome formulations

Anita Dudek, Hanna Pruchnik, Paulina Strugała-Danak

Department of Physics and Biophysics, Wrocław University of Environmental and Life Sciences

Anita Dudek: anita.dudek@upwr.edu.pl

The aim of the work is to analyze the potential enhancement of the biological activity, particularly the anticancer potential, of flavonoids with chlorine and bromine atoms by creating encapsulated liposomes as potential carriers of bioactive compounds. Flavonoids, as a group of natural compounds, exhibit a range of health-promoting properties including anti-inflammatory, antidiabetic, antiseptic, and anticancer properties [1]. The structure of flavonoids does not allow for the complete utilization of their therapeutic potential. Poor solubility, short circulation time in the bloodstream, low stability, and bioavailability significantly limit their utilization. One potential modification of flavonoids is the synthesis of flavones, for example, with chlorine and/or bromine atoms [2].

Liposomes, as carriers of active substances, are widely used due to their biocompatibility, non-toxicity, and relatively low production cost. Studies indicate that liposomes can be effective carriers for polyphenolic compounds of natural origin, including flavonoids [3]. In order to encapsulate selected compounds in liposomes and form a functional carrier, it is essential to conduct a comprehensive characterization of the physicochemical and biophysical properties of the flavonoid-lipid carrier system and characterize their anticancer properties (Fig. 1). The employment of methods such as Raman spectroscopy (FT-Raman), infrared spectroscopy (ATR-FTIR), spectrofluorimetric methods, molecular dynamics (MD) scanning electron microscopy and transmission electron microscopy (SEM, TEM) will permit the determination of precise interactions at the lipid bilayer level. Furthermore, a variety of biological techniques, including flow cytometry and western blot, will enable the assessment of the behaviour of formed nanoliposomes in biological systems and toxicity along with anticancer properties towards canine cancer cells.

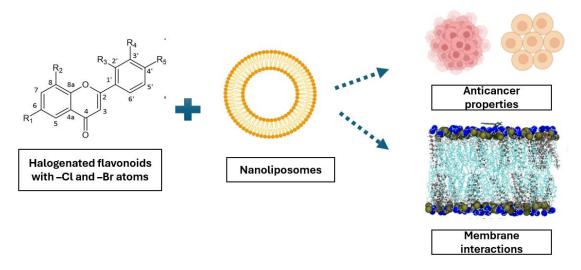


Fig. 1. Graphical abstract

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Keywords: halogenated flavonoids, encapsulation, liposomes, drug delivery, anticancer properties

Flow capacitive deionization – process introduction

Justyna Nowicka

Department of Chemistry, Wroclaw University of Science and Technology

Justyna Nowicka: justyna.nowicka@pwr.edu.pl

Flow capacitive deionization (FCDI) (Fig. 1) is a relatively new separation technology, a modification of capacitive deionization (CDI). CDI is based on causing ions movement in an electric field. On their way towards oppositely charged electrode, ions are segregated by ion exchange membranes (cation – CEMs and anion – AEMs). Those thin films made of modified polymers pass through only counter-ions (species charged oppositely to ionic groups in the membrane). Then ions are adsorbed on the electrode material, usually activated carbon (AC). It allows both solvent purification and dissolved substances recovery. Some of the used energy can be recovered in the desorption process [1]. CDI is a batch process because it has to be stopped for electrode regeneration. However, in FCDI the solid activated carbon is replaced by suspension of AC. Therefore, the process may be carried out in a continuous way. FCDI seems to be an effective and environmentally friendly tool for resources recovery [2].

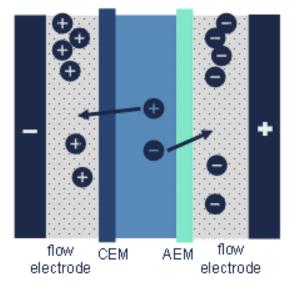


Fig. 1. The concept of flow capacitive deionization

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Keywords: flow capacitive deionization, ion exchange membranes, electromembrane processes, metals separation

Probiotic strains as support for the host against Salmonella infections

Ewa Carolak

Wrocław University of Environmental and Life Sciences, The Faculty of Veterinary Medicine, Department of Biochemistry and Molecular Biology, Norwida 25, 50-375 Wrocław

Ewa Carolak: ewa.carolak@upwr.edu.pl

Salmonellosis, a prevalent cause of foodborne illness, not only impacts public health but also presents a significant economic burden due to frequent infections in livestock. The pathogenesis of Salmonella infection depends on initial stages, particularly effective adhesion and invasion, wherein the pathogen attaches to host epithelial cells and colonizes the intestinal mucosa. This infectious process unfolds within a complex microbial environment comprising the host's microbiome, consisting of countless microorganisms [1]. The interaction between pathogens like Salmonella and the host occurs among a diverse microbial milieu, influencing the course and severity of infection. Among these microorganisms are probiotics - non-pathogenic microbes known for their potential health benefits. Probiotics exert multiple effects on infection outcomes, including inhibiting the growth of pathogenic bacteria, modulating the immune response, and reinforcing the intestinal barrier [2]. A noteworthy mechanism by which probiotics exert protective effects is through adhesion to the intestinal mucosa, which can impede the binding of enteropathogens to host cells. This competitive binding can prevent the establishment of infection by pathogens. Lactic acid bacteria (LAB) represent a well-studied group of probiotics, encompassing over 250 species of Lactobacillus known for their diverse beneficial properties in the gut environment [3]. Another prominent probiotic bacterium is Escherichia coli Nissle 1917 (EcN), a gram-negative rod-shaped bacterium belonging to the same family (Enterobacteriaceae) as Salmonella. EcN has garnered attention for its ability to compete with enteropathogens and has been utilized in various therapeutic interventions, including the management of diarrheal illnesses [4]. Understanding the interplay between probiotics, Salmonella, and the host microbiome is crucial for developing targeted interventions to mitigate Salmonella infections. By explaining the specific mechanisms through which probiotics confer protection – such as adhesion-mediated competition for binding sites and modulation of host immune responses – novel strategies can be devised to harness the potential of probiotics in combating foodborne pathogens and enhancing livestock health.

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Keywords: probiotic bacteria, adhesion, fimbria, Salmonella, microbiome

MXenes for electrochemical reduction of carbon dioxide

Marta Posadzy, Karolina Kordek-Khalil, Piotr Rutkowski

Department of Process Engineering and Technology of Polymer and Carbon Materials, Faculty of Chemistry, Wrocław University of Science and Technology

Marta Posadzy: marta.posadzy@pwr.edu.pl

The constantly growing emissions of carbon dioxide will undoubtedly result in the deterioration of natural environment and atmosphere. A promising strategy for reducing carbon dioxide concentration in the atmosphere is to convert CO₂ into valuable chemicals and fuels such as CO, HCOOH, CH₃OH, etc., thus closing the carbon cycle [1]. Electrochemical reduction of CO_2 has many advantages; for example, it can be performed at ambient temperature and pressure, and the electricity needed to drive the reaction can be supplied from renewable energy sources. To drive the desired chemical transformations with high selectivity and energy efficiency, an effective electrocatalyst needs to be used. There are several fundamental and practical challenges in the design of electrocatalysts for CO₂ reduction. The process involves complex reaction pathways and it is often competing with hydrogen evolution reaction [2]. Metal electrocatalysts, such as copper and gold have been shown to reduce CO₂ into valuable products. However, they demand high overpotentials, and have low stability and selectivity [3]. Therefore, it is necessary to develop efficient noble-metal free electrocatalysts. Two-dimensional (2D) materials are promising electrocatalysts due to their unique electronic and structural properties, excellent electrical conductivities, high atom utilization and large specific surface area [4]. A particularly interesting kind of 2D material is MXene, a relatively new class of materials, first synthesised in 2011. MXenes consist of atomic layers of early transition metal bonded with carbon or nitrogen, and interspersed with surface terminations, e.g., hydroxyl, fluorine. These materials exhibit excellent properties, including chemical and mechanical stability and tunability of surface chemistry [5]. Applications of MXenes as electrocatalysts and photocatalysts have been recently investigated. Several works have focused on their catalytic effect in electrochemical reduction of CO₂, mostly investigating their activity using DFT calculations. Based on these calculations, several MXenes are promising CO2 reduction electrocatalysts, and experimental studies are needed to confirm their potential.

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Keywords: MXenes, 2D materials, electrocatalysis, electrochemical reduction of CO2

Fragrance compounds - synthesis, evaluation, and potential applications

Kinga Baberowska^{1, 2}, Alicja K. Surowiak², Daniel J. Strub²

¹ Department of Analytical Chemistry and Chemical Metallurgy, Wrocław University of Science and Technology ² Department of Chemical Biology and Bioimaging, Wrocław University of Science and Technology

Kinga Baberowska: kinga.baberowska@pwr.edu.pl

The flavour and fragrance industry relies on a wide range of raw materials to create a diverse group of products. Each product is made up of many different chemicals that often mix together in complex ways. The industry can be divided into four main categories: natural, nature-identical and synthetic or artificial. These categories encompass a wide variety of substances used to impart taste and scent to consumer goods [1].

The fragrance industry is experiencing dynamic growth on a global scale, primarily driven by synthetic fragrances [2]. Despite this dominance, numerous commercially available fragrances face limitations in their usage and are undergoing withdrawal due to associated toxic effects. This trend underscores the urgent need for safer and more sustainable alternatives in the market.

One of the main research goals is to create new chemical compounds with aromatic profiles resembling flower essences. Using the Bargellini reaction, acid derivatives (intermediate derivatives) were synthesized. These intermediates were then combinatorically synthesized with mixtures of alcohols catalyzed by DCC (N,N'-Dicyclohexylcarbodiimide) and DMAP (4-Dimethylaminopyridine), yielding a diverse range of esters. Gas chromatography with an olfactometric detection (GC-O) was used to evaluate the aromatic properties of the synthesized ester mixtures. After comprehensive GC-O analysis, esters showing pleasant aromatic properties were assigned for further study. The individual synthesis of selected esters is currently ongoing, which represents the next stage of research.

After completion of the synthesis process, the biological efficacy of the newly synthesized phenolic derivatives, characterized by distinctive odour profiles, will be examined. Comprehensive assessments will include an evaluation of their antimicrobial activity along with an assessment of their cytotoxicity potential towards human cells.

The synthesis of these novel compounds not only addresses an underexplored research domain but also presents promising prospects for commercialization. Furthermore, continued research endeavours in this topic hold the potential to bridge existing knowledge gaps and facilitate the acquisition of novel insights.

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Keywords: fragrance industry, synthetic fragrances, chemical compounds, aromatic properties, biological efficacy

Does industrial activity affect the levels of selected heavy metals in soils in the allotment gardens of Wroclaw?

Dariusz Gruszka¹, Małgorzata Wilusz-Nogueira¹, Szymon Jędrzejewski¹, Magdalena Bednik¹, Jarosław Szadorski¹, Anita Jandy¹, Anna Fleszar¹, Bogna Kosyk¹, Joanna Magiera-Dulewicz², Kamila Twardowska²

 ¹ Institute of Soil Science, Plant Nutrition and Environmental Protection, Wrocław University of Environmental and Life Sciences
 ² Department of Plant Protection, Wrocław University of Environmental and Life Sciences

Dariusz Gruszka: dariusz.gruszka@upwr.edu.pl

Allotment gardens, often referred to as small family gardens, are a popular place of recreation for urban residents in Poland. In addition, they are also used for growing vegetables and fruits. However, there is a risk of problems associated with vegetables taking up potentially toxic elements that contaminate garden soil, which carries health risks for those who eat the vegetables. In addition, contamination of garden soils can lead to a reduction in the population and diversity of organisms living in such conditions.

The purpose of this study was to investigate the content of selected trace elements (Cu, Pb, Cd and Zn) in garden soils located in nine allotment garden complexes in Wroclaw. Soil samples were taken from various locations in the city, from a depth of 0–30 cm, from a total of about 110 locations. Heavy metal contamination was determined for each plot. It was Cd, Pb, Cd, and Zn. Total forms were determined by soil mineralisation with "aqua regia", which corresponds to the content of trace elements close to the total. The results showed that in some areas garden soils are low/heavily contaminated with elements such as cadmium 1–6 [mg/kg], lead 19–401 [mg/kg], copper 24–322 [mg/kg] and zinc 101–3464 [mg/kg], exceeding the permissible values according to Polish legislation. The permissible levels of trace elements for agricultural and horticultural soils in Polish legislation are: for Cd to 3 [mg/kg], for Pb to 250 [mg/kg], for Cu 150 [mg/kg] and for Zn 500 [mg/kg].

Particularly high concentrations of these elements have been found at the site of Hutmen, anon-ferrous metallurgy plant that in the past emitted significant amounts of metal-bearing dust. As a consequence of industrial plant operations in the 1970s and 1980s, as a result of intensive emissions of metallurgical dust, trace elements reached the soils with the deposition of these dusts, causing their accumulation in soils.

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Keywords: garden soils, allotments, heavy metals, contamination

Polylactide coated homogeneous structures based on hyaluronic acid-sodium alginate

Maciej Grabowski, Anna Trusek

Department of Bioprocess Micro and Nanoengineering, Wrocław University of Science and Technology

Maciej Grabowski: maciej.grabowski@pwr.edu.pl

Using a controlled release drug carrier is an innovative solution for treating topical infections, especially in dentistry, skin diseases and open wounds. Hydrogels are often studied because of their biodegradability, biocompatibility, ability to adsorb large amounts of drugs (especially those with hydrophilic properties) and ability to form structures of any shape and size. Sodium alginate (SAL) and hyaluronic acid (HA) based hydrogels have gained considerable attention as drug carriers due to their biocompatibility and biodegradability [1]. Poly(lactic acid) (PLA), a biocompatible polyester, offers further opportunities in drug delivery [2]. During this research, drug release tests were carried out from the HA–SAL capsules, coated with PLA. The procedure of the coating of capsules is presented in Figure 1. The synergistic combination of alginate, hyaluronic acid and poly(lactic acid) has great potential for the creation of homogeneous structures that are capable of the controlled release of antibiotics.

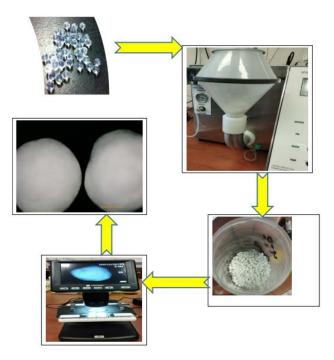


Fig. 1. The procedure for coating capsules (PLA-HA-SAL)

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Keywords: hyaluronic acid, sodium alginate, poly(lactic acid), hydrogels, drug carriers, antibiotic release

New Multidimensional Data Structure for Vario-scale Spatial Model Representation

Amin Gholami

Wrocław University of Environmental and Life Sciences, Institute of Geodesy and Geoinformatics, Grunwaldzka 53, 50-357 Wrocław, Poland

Amin Gholami: amin.gholami@upwr.edu.pl

This thesis discusses the representation of the scale dimension using tGAP/SSC-DHE, emphasising its role in creating vario-scale representations. It outlines the process of integrating the scale dimension as the third dimension in a 2D map before transitioning to 3D or 4D maps. DHE is introduced as an effective data structure for this approach, maintaining crucial connections across different levels of detail and offering enhanced topology. Its strength lies in the ability to modify specific parts of the model while retaining a clear structure, thanks to well-defined operators such as Euler operators. This method provides a versatile framework for representing complex spatial data, allowing for detailed analysis while preserving overall coherence. Through practical implementation, it demonstrates the potential for improved visualisation and understanding of multi-dimensional spatial relationships.

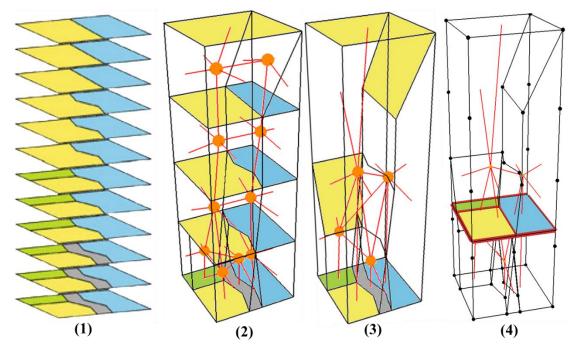


Fig. 1. Reconstruction tGAP/SSC by DHE data structure

Here's where our approach differs. We have developed an innovative data structure that overcomes these limitations. As shown in Fig 1.2 by introducing vertical lines between layers, we transform a 2D map into a 3D model. Additionally, as shown in Fig 1.3 we use inclined lines to ensure smooth transitions between different levels of detail. By using the slicing method as shown in Fig 1.4. This innovation allows us to create a virtually unlimited number of maps at varying scales, giving users the flexibility to explore spatial data like never before (Fig 1.1).

Keywords: vario-scale, LOD, multi-dimensional modelling, topology, DHE

Changing the paradigm of designing streets in our cities

Anastasiia Zhokhova

Department of Urban Planning and Spatial Management, Wrocław University of Science and Technology

Anastasiia Zhokhova: anastasiia.zhokhova@pwr.edu.pl

Before the car's emergence, streets served as public spaces and provided vivid urban life. Since the end of the previous centuries, cars began to play a key role in our cities and became a defining indicator for street design. Therefore, streets turned into roads and highways. Even though today's vision and goals of urban planning have transformed to measure up sustainable approach to mobility, the principles of street design have not changed significantly. Moreover, street reconstructions often do not comply with upper-level strategy forming documents, policies and integrated conceptions, nor do they address modern needs and challenges.

The participation process begins to be frequently used for designing public spaces and for planning district and area development concepts but is still rarely used when it comes to street design. On the one hand, we can observe an increasing number of participation examples in street design and a gradual change of the paradigm to street design in some European cities, for instance, Barcelona, Paris, Amsterdam, Delft, Antwerp, Vienne etc. On the other hand, these changes remain non-systematic and are not widely spread, especially when it comes to Ukrainian and Polish cities, which are the main focus of the research. Street design is commonly developed by road engineers, usually without in-depth research into the needs and experiences of people who live and function on that street. As a consequence, the result may not meet the expectations, the design decisions may be misused, unforeseen conflicts may emerge, and the costs and time invested into street design do not pay off.

Street reconstructions are expensive investments, the result of which remains for decades. Furthermore, they do not end with their commissioning as the exploitation phase follows. However, street design is still not treated as an integrated and continuous project that needs proper maintenance and analysis as well.

Inspired by the IT branch with its project management framework application, thorough in-depth UX research, minimum viable product (MVP) testing system, and iterative and continuous improvement approach engaging users at almost all stages of the project life cycle, I suggest worthy to learn from, adapt and use these practices and approach in street design.

Using the project management framework, we can smoothly include the participation process that will involve street residents, visitors and other stakeholders to develop a clear vision for the street and identify the needs of its users. The facilitation process should be carefully organised to provide optimal outcomes. The environmental and social impact should be considered a high priority. Along with the direct involvement of the stakeholders, just as important is to conduct user experience research and explore behavioural patterns paying attention to how different categories of people use the infrastructure. It will help to adopt a proper infrastructure design. Design decisions should be tested with available tools of tactical urbanism providing a minimum viable product for assessment. After completion of construction, the project analyses should be committed considering felicitous decisions which are nice to apply for the next projects and fault decisions which should not be repeated in the next projects. But it is still not the end of the project. We can engage street users to help in the proper functioning and maintenance of the street, for instance, by reporting issues such as conflict or unconsidered zones, deterioration of the surface or infrastructure damages, and expressing their needs for further changes on the street, etc.



Fig. 1. Visualisation of the street reconstruction process in a project management framework with the adoption of the best IT management practices

Such an approach to street design can ensure a real inclusive process that considers all stakeholders harmonising their needs with sustainable principles, offering justified decisions and high-quality street projects, and providing constant improvement for current and further projects.

Keywords: human-centred planning, sustainable urban mobility, self-sufficient cities, bioclimatic design, project management

Chosen realisations of multi-family buildings in Wrocław after the year 2000 – qualitative research of flats

Magdalena Odziemek

Department of Architecture, Wrocław University of Science and Technology

Magdalena Odziemek: magdalena.odziemek@pwr.edu.pl

Residential development architecture is one of the fastest-growing branches of architecture in recent years. The topic of housing also concerns every person, and as research shows, a bad housing situation is one of the three biggest problems for Poles [4]. As Jan Chmielewski wrote "The choice of place to live – settlement – was and is one of the most important life decisions that a person makes during his earthly existence. (...)" [1].

2020 was a particularly important year for the housing market. A record number of apartments (in 31 years) was put into use in Poland – it amounted to over 220,000. This result was almost 7% higher compared to the previous year and over 19% compared to 2018. These numbers placed Poland first in Europe in terms of the number of apartments built in the country per 1,000 inhabitants. At the same time anyway, our country was still in one of the last places in terms of apartments available per 1,000 inhabitants.

Also unexpected situations later, such as the Covid-19 pandemic, the war beyond Poland's eastern border or a very rapid increase in inflation, and as a result, an increase in the prices of construction materials and a decline in the credit-worthiness of Poles, resulted in decreasing interest in purchasing real estate among Poles. Due to these and other factors, even more importance is attached to the decision of buying an apartment. In March last year, the average sale of developer apartments in the 7 largest cities was 48% lower than in March last year. Meanwhile, in March this year compared to last year, we had to pay an average of almost 23% more per square meter of apartment in these cities [3].

Different questions appear in this situation. Has the quality of newly designed and built apartments offered on the market, changed? Do people pay more attention to the type of apartments they buy and what guides their choices? What buildings and apartments are being delivered by development companies that are the main investors in Poland, in the largest cities of our country and how it looked like on the map of Wrocław [2]?

In my dissertation, I try to answer these and similar questions, mainly by analysing the residential real estate market in Wrocław after 2000, in terms of the number, size, location and other aspects of development investments. Then I perform POE (Post-Occupancy Evaluation) studies on selected realizations and assess their quality in terms of generally accepted design standards as well as from the point of view of their everyday users [5].

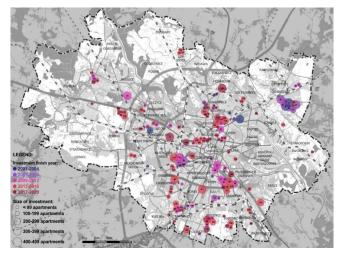


Fig. 1. Number, size and location of development investment put into use in Wrocław in particular years between 2000 and 2020. Author: Magdalena Odziemek

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Keywords: flats, real estate market, Wrocław, development companies, residential architecture

Global Navigation Satellite System role in atmosphere monitoring

Adam Cegła

Institute of Geodesy and Geoinformatics, Wrocław University of Enivronmental and Life Sciences

Adam Cegła: adam.cegla@upwr.edu.pl

The original concept of satellite observation was initially focused on enhancing the navigation capabilities of military forces. However, with the passage of time and the emergence of successive counterparts to the US GPS system (such as Galileo, Beidou, and GLONASS), the technology became accessible to civilians and found its way into many aspects of everyday life. It is now difficult to imagine routine activities without digital maps on electronic devices or the ability to instantly locate ourselves, despite the occasional inaccuracies.

The inaccuracy of satellite systems (GNSS) is rooted in the physical properties of the atmosphere and the environment of the signal receiver. Generally, efforts are made to correct system flaws using available tools, but this is not always the case with GNSS observations. Surprisingly, their unexpected beneficiary is the meteorological environment.

The physical properties of the electromagnetic wave sent by the satellite transmitter make it susceptible to deflection, which is detected by the GNSS receiver in the form of signal transmission time. This deflection occurs due to variations in atmospheric pressure, humidity, and temperature – parameters crucial to the current state of the atmosphere and any weather phenomena.

This makes GNSS stand out as an unbiased, reliable, cheaper, and ground-independent substitute among data sources, with weather stations and radiosondes playing a major role. Based on GNSS observations, it is possible to construct an accurate model of a storm or tropical cyclone. With sufficient data, it is also feasible to model the atmosphere over an entire country or continent, and subsequently assimilate the data into Numerical Weather Models. In the long run, this also implies enhanced weather forecasts and a deeper understanding of perennial phenomena such as El Niño or La Niña.

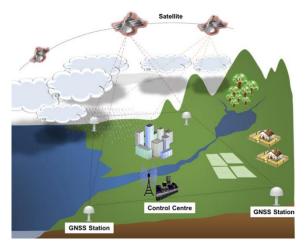


Fig. 1. GNSS monitoring of the atmosphere

Literature

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Keywords: atmosphere, GNSS meteorology, Numerical Weather Models

Modelling of travels in agglomeration transport networks

Michał Zawodny

Department of Road, Bridges, Rails, and Airports, Faculty of Civil Engineering, Wrocław University of Science and Technology

Michał Zawodny: michal.zawodny@pwr.edu.pl

In communication-related construction, as in the case of buildings, initial assumptions must be made and loads must be collected. Loads in road or rail construction will be the streams of travellers. In the case of renovation or reconstruction of existing infrastructure, it is possible to take traffic measurements and convert them into the number of axles that will affect the roadway structure in the assumed time horizon. However, the situation becomes more complicated when one goes beyond simple road renovations and modifies the entire transportation network with new connections, or the construction of new tram routes. Then ordinary traffic measurements are not enough. It is necessary to estimate how many travelers will choose the planned means of transportation, and which option will attract the most residents to use public transportation. How to design the infrastructure so that it will best perform its function, so it will be the most favourable from the point of view of cost-benefit analyses? For this purpose, transport models are needed.

Transportation models need preliminary data on traveller movements [1]. These are not easily measured values such as the number of vehicles of a particular category on a particular cross-section of road. Originally, surveys were used for this purpose; in Poland, with low responsiveness, surveys are difficult to conduct. In order to obtain detailed data on traveller movements, Big Data sources began to be used, and the data sources in transportation are increasing, as shown in Fig. 1. In order to obtain detailed data on traveler movements, Big Data sources began to be used, and the data sources began to be used. Due to the lack of a systematized methodology for combining databases from disparate Big Data sources, mainly based on modern technologies (mobile network, Bluetooth, smart card data, etc.), it is necessary to create a method for combining them, which will not be an ad hoc solution as in current research [2, 3]. The agglomeration that has the selected 11 sources does not exist, therefore, in this work, an O-D matrix was simulated for a theoretical agglomeration. Due to the breadth of the work, the doctoral dissertation focuses on only one part of the four-stadium model, the planned movement potentials alone. The method will take into account the bias of each source, such as socio-demographic data, and complete the O-D matrix, which has gaps and unreliable data. A neural network will be used for this purpose.

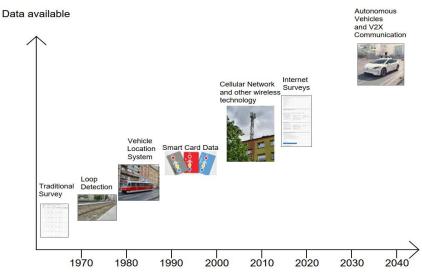


Fig. 1. Increase in data sources in transportation

Literature

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Keywords: transport modelling, O-D matrix, big data, transportation, agglomeration

Efficient nitrogen preservation in organo-mineral fertilizers

Krzysztof Trzaska, Filip Gil, Dawid Skrzypczak, Katarzyna Chojnacka

Department of Advanced Material Technologies, Wrocław University of Science and Technology,

50-370 Wrocław, Lower Silesia, Poland

Krzysztof Trzaska: krzysztof.trzaska@pwr.edu.pl

Faced with the challenges of increasing demand for food production and limited farmland, studies to help reduce nitrogen (N) losses in agricultural practices have been conducted. The study used sewage sludge as a valuable and mostly loose nitrogen source. Wastewater treatment plants (WWTPs) in the EU produce more than 10 million tons per year of dry sludge [1]. It is converted into organo-mineral or organic fertilizer by thermal, chemical and biological methods. The main thermal method is drying, both using electricity and natural sources (sun). In many cases, it is dried under inappropriate conditions (too high temperatures), leading to significant nitrogen losses. Since nitrogen is the basic yield-forming component of fertilizers, its loss is extremely unfavourable for further agricultural use [2]. Seven types of air drying at temperatures of 10–150 degrees Celsius and for 5 h–20 days and other thermal methods (combustion, pyrolysis) were compared. Chemical hydrolysis was used in the later stages. It is widely used for waste management and in the fertilizer industry. The neutralization process of the resulting hydrolysate is also important due to the level of nitrogen losses, as shown in Fig. 1. At the same time, one-step management methods using CaO dehydration/granulation methods also gain significance. Due to the simplicity of application to different types of materials, they are considered a rapid technology for introduction and use. Composting, as a widely used biological technique for waste disposal, also leads to significant nitrogen losses. To minimize them, kitchen waste additive during drying was used according to Krasowska et al. (2023) [3].

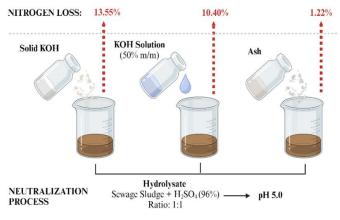


Fig. 1. Nitrogen losses during neutralization process

The work led to a comparison of different types of technologies used in valorization and waste treatment. In chemical processes, pH has been identified as an extremely important factor. Acidic environments retain nitrogen more effectively than alkaline conditions, highlighting the need for careful pH control during processing. Although thermal methods are effective in reducing the moisture content, volume and microbial activity of sludge, they also cause significant nitrogen depletion, requiring an optimum between drying efficiency and nutrient retention. Composting is an advantageous approach that provides a balance between nutrient recovery and safety, although minimizing nitrogen loss remains a challenge and requires optimal conditions for efficiency.

This work was financed by the Horizon 2020 Research & Innovation Program of the European Union under grant agreement No. 696356, the Executive Agency for Higher Education, Research, Development, and Innovation Funding, UEFISCDI (Romania), the National Center for Research and Development, NCBR (Poland), AEI (Spain), and the Ministry of Agriculture and Forestry, MMM (Finland) and by the National Science Center, under project no. MINIATURA7: 02NA/0024/23.

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Keywords: sewage sludge, resource recovery; environmental impact; treatment optimization; sustainable agriculture

High-Torque Pernament Magnet Synchronous Motor in Lower Limb Exoskeleton

Michał Cichowicz

ZUT Doctoral School, Depertment of Electrical Machnies and Drives, Faculty of Electrical Engineering, West Pomeranian University of Technology in Szczecin

Michał Cichowicz: michal.cichowicz@zut.edu.pl

In this paper the novel concepts of high torque permanent magnet synchronous machines (HTPMSM) for biomechanical constructions applications will be presented. The main construction of the machine is a modified PMSM. It will be extended with different types of transmissions: magnetic gearbox, harmonic gearbox, or both. Additionally, the permanent magnets (PMs) in motor and gearbox will be placed in a Halbach array. The main goal of the research is to obtain as high torque on a machine's shaft as possible with relatively small size of a motor and possibly high rotational speed for reaching a smooth movement of biomechanical constructions.

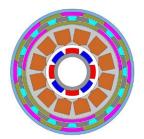


Fig. 1. An example of a reluctance machine with outer magnetic gearbox implementation

Initial conditions

In the beginning of the design, it is necessary to define the initial conditions for the biomechanical drive:

- a user of the biomechanical construction will not overcome a body weight of 150 kg,
- a motor outer diameter will not overcome 80 mm,
- a total motor construction needs to be relatively light for not charging the entire exoskeleton construction and human body,
- a motor needs to be controlled with wide speed range,
- the PMs will be placed in a Halbach array.

These conditions enable the selection and optimization of the electrical and mechanical machine that will ultimately be used – this is the topic of the final version of the paper.

Gearbox simulation tests:

Figure 2 presents first simulational magnetic gearbox tests. It shows that the torque of the gearbox is relatively big and equal around 5 kNm.

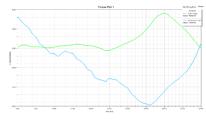


Fig. 2. Magnetic gearbox torque plot

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Keywords: permanent magnet motors, magnetic gears, mechanobiology, wearable robots, lower limb exoskeleton

Active Disturbance Rejection Control Based on Neural Model Applied for Two-mass System

Grzegorz Kaczmarczyk

Department of Electrical Machines, Drives and Measurements, Faculty of Electrical Engineering, Wrocław University of Science and Technology

Grzegorz Kaczmarczyk: grzegorz.kaczmarczyk@pwr.edu.pl

In modern industry almost every single factory is based on modern electric drive solution. Complex technological processes often require high dynamics and robustness combined with low maintenance and reduced costs of the used electric systems. Moreover, sophisticated technological methods also force the need to use a complex mechanical structure, which is a huge impediment with regard to control facility and accuracy. A two-mass system is considered as a one of the most common mechanical part of the drive unit. It is widely used in many fields of science and industry (e.g., electric cars, conveyor belts, wind turbines, positioning systems, etc.). For the sake of scientific research, a model mentioned above can be described as two electric motors connected together with a long (elastic) shaft. A wide variety of possible applications, a huge range of hypothetical changeable environmental conditions and issues related to the identification process, lead to increasing the number of applications related to robust and adaptive control methods. The main goal is to compensate any uncertainties of the drive (e.g., changes of static/dynamic friction values, fluctuations of parameters of the object, additional shaft flexibility or backlash) occurred during exploitation. In addition, restrictive requirements deal with reducing the number of measurement sensors (low costs, system reliability). In order to satisfy above mentioned requirements of the modern electric drive with sophisticated mechanical part, an Active Disturbance Rejection Control (ADRC) is currently tested. The main concept of the ADRC is to treat both external and internal disruptions (e.g., additional load torque, changes of friction, elasticity of the shaft) as an additional disturbance. The current value of the disruption is estimated on-line with the use of the Extended State Observer (ESO). Afterwards, it is subtracted from the initial form of the control signal produced by the controller. Furthermore, the main assumption of the ADRC states that the exact plant model does not need to be known, as it can be presented in the form of multi-integrator block. Described approach makes the ADRC algorithm a promising control strategy. It ensures high control accuracy and excellent dynamic properties. The doctoral dissertation is focused on the modified ADRC algorithm. The main idea of the thesis is to improve the robustness against drive parameters changes. It can be achieved with the adaptive capabilities of a neural model. The conducted works will be divided into two main parts (with two principal variants of the ADRC structure). The first one involves a standard ADRC method, developed by prof. Han [1]. It assumes the presence of a Tracking Differentiator (TD) block applied with the non-linear feedback. The purpose of the TD is to shape the desired dynamics of particular state variables, which are then passed along to the further part of the control system. Presented approach gives a possibility to substitute the ADRC controller block with similar, non-linear adaptive or robust structure (e.g., Radial Basis Function Neural Network or Fuzzy Logic Controller). The second method is based on the ADRC variation developed by the research team headed by prof. Brock [2]. The main assumption of presented solution states that the whole ADRC controller is based on the two-mass system model. The approach proposed by prof. Brock does not require the use of the TD block, which significantly simplifies the numerical complexity of the algorithm. Moreover, it assumes that the load side speed measurement is the only available physical signal. The second part of the doctoral dissertation involves the Extended State Observer improvement. All of the works included in the second part of the works are to increase the robustness of the system with regard to ESO implementation. The main contribution of the doctoral dissertation is to make an ADRC algorithm more robust and invulnerable to a sudden change of the plant parameters. Besides, a low numerical complexity makes the ADRC a feasible solution in terms of an accurate, low-cost control system deployment. Thus, it is important to increase its resilience on the implementation inaccuracies. The doctoral thesis involves elaboration of the current state of the art overview in the field of two-mass electric drive systems control and ADRC technique, development of a novel ADRC algorithm improvement with the use of neural model, application of meta-heuristic algorithms in tuning process, carrying out numerical and experimental tests of the proposed approach and evaluation of the obtained results.

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Keywords: electric drives, ADRC, neural networks, artificial intelligence, automatics

Toward sustainable rail transport: a comprehensive approach for identifying and mitigating environmental impacts

Julia Milewicz, Tomasz Nowakowski, Grzegorz M. Szymański

Institute of Transport, Poznan University of Technology

Julia Milewicz: julia.milewicz@doctorate.put.poznan.pl

Despite being considered one of the most environmentally friendly modes of transportation, rail transport still faces challenges associated with train-wildlife collisions and the fragmentation of natural habitats, directly leading to ecosystem impoverishment, which is one of the main threats identified by environmental organisations and International Union of Railways [1]. The application of appropriate mitigating actions to prevent biodiversity loss is one of the tasks covered by the Sustainable Development Strategy [2]. To mitigate these negative aspects of rail transportation, both passive methods, such as wildlife overpasses or underpasses, and active methods, which do not physically prevent access to the tracks but emit deterrent signals upon train approach, are being used [3]. However, due to the lack of a universal method for identifying and characterising direct threats to wildlife and selecting appropriate mitigation measures, the actions of stakeholders may be chaotic or impractical. The presented procedural model allows effective data management and facilitates decision-making with regard to necessary solutions, considering external and internal factors. With this method, it will be possible to systematically implement solutions to mitigate the impact of the railway on the ecosystem by designating hotspots, i.e., locations prone to collisions between trains and wildlife and loss of biodiversity due to vehicle operations. By analysing the information in a structured way and selecting appropriate countermeasures to the situation, together with methods for evaluating their effectiveness, can become part of the environmental reports regularly carried out by railway undertakings, infrastructure managers, and environmental organisations. This allows for rational and environmentally friendly decisions on both modernisation changes and the development of the rail network. An integral part of the model is also a set of implementation recommendations for stakeholders. In this way, the tool serves the strategy of sustainable development of rail transport in a universal manner.

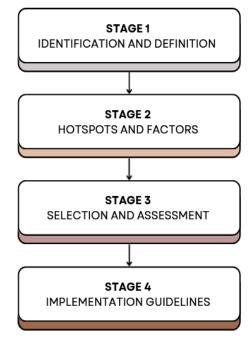


Fig. 1. Simplistic approach to analysing the phenomenon, selecting and implementing relevant mitigation measures (as a part of an overall method)

Literature

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Keywords: ecology, rail transport, mitigating environmental impacts, assessment method, sustainability

All the shades of H₂O₂-sensitized TiO₂

Anna Gibas, Agnieszka Baszczuk

Department of Mechanics, Materials and Biomedical Engineering, Wrocław University of Science and Technology

Anna Gibas: anna.gibas@pwr.edu.pl

The concept of "colored titanium dioxide" (violet, blue, green, yellow, orange, or black) as visible-light active photocatalysts is widely accepted. This statement bases on the understanding that the visual colours exhibited by TiO_2 are results from intrinsic defects, such as various oxidation states (Ti^{3+} , Ti^{2+}), oxygen vacancies and/or other defects, that create additional electronic states in the TiO_2 bandgap that alter their optoelectronic properties [1, 2].

In this study, we verify this claim with respect to TiO_2 that has been synthesized using hydrogen peroxide. Upon the contact of H_2O_2 with titania, hydroxyl groups are formed on the surface of the Ti-precursor which then transform in the excess of the H_2O_2 to the peroxo groups [3]. The color of reaction mixture changes instantly and ranges from green, through yellow, and red to brown depending on the type of the peroxo groups (linear Ti-OOH, Ti-O-O-Ti, and triangular TiO₂) and their concentrations [3–5]. The colour of the dried H_2O_2 -treated TiO₂ appear yellow to the naked eye [6]. Usually, peroxo and superoxo complexes serve as an essential intermediate step to achieve hydrated crystalline TiO₂ phases. But both types of groups exhibit thermal sensitivity [7] and decompose when TiO₂ is annealed which turn the TiO₂ to white. In this study, we decided to prepare TiO₂ without high temperature treatment to ensure the presence and stability of all peroxo and superoxo groups after powder drying. As-prepared yellow TiO₂ powder was tested then for degradation of methylene blue under visible light. During the test H_2O_2 -sensitized TiO₂ becomes blue upon adsorption, yellow after catalysis and for some incomplete degradation processes – green. For all cases, it recovers to yellow after the laser treatment. And all things considered, TiO₂ is a vivid material putting colors into photocatalytic process.

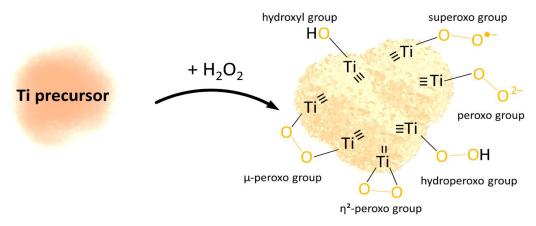


Fig. 1. Scheme of the H2O2-sensitized TiO2

Literature

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Keywords: titanium dioxide, hydrogen peroxide, yellow titanium dioxide, visible light activity

Listening to semiconductors: photoacoustic spectroscopy – a powerful technique to investigate semiconducting samples

Kamil Misztal

Department of Semiconductor Materials Engineering, Wrocław University of Science and Technology

Kamil Misztal: kamil.misztal@pwr.edu.pl

Photoacoustic spectroscopy (PAS) is a powerful technique to investigate semiconductors and determine some of their basic properties, e.g., energy gap [1], thermal conductivity [2], and thermal diffusivity [1, 3]. This method is based on light absorption by the material under consideration and detecting gas pressure oscillations. When the modulated light hits the sample enclosed in a specially designed photoacoustic (PA) cell the sample is periodically heated. This heating is caused by non-radiative relaxation processes taking place in the material after light absorption. Next, the sample releases heat to surrounding gas typically air at atmospheric pressure in this method. Periodically releasing heat into the air causes oscillations because of thermal expansion which are actually sound. Hence, it is possible to measure this sound with a proper microphone. The above description of generating the PA signal is schematically presented in Fig. 1.

Notably, PAS does not require special preparation of samples and facilitates the measurement of samples challenging to study using conventional absorption/transmission techniques due to factors such as high light scattering, opaqueness, or sample state (e.g., powdered or liquid form) [4–6]. The key advantage of PAS lies in its reliance on sound detection rather than light, ensuring consistent sensitivity across the spectral range without the need for different photodetectors.

In my presentation, I will focus on the PAS principle. Moreover, I will show how the PA signal is generated by an example of MoS_2 and I will present how to interpret obtained spectra.

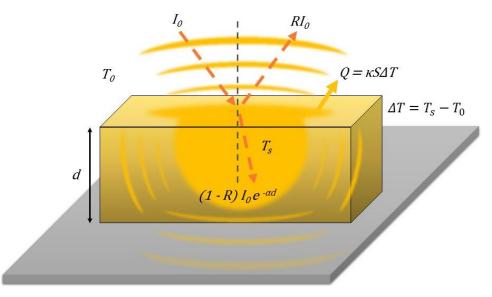


Fig. 1. Scheme of the heat generation and its release from the sample in the PAS technique. Orange arrows indicate modulated light and the dark yellow waves and the area indicate heat

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Keywords: photoacoustic spectroscopy, signal generation, MoS₂

The potential of greenery in alleviating discomfort related to road infrastructure – a literature review

Agata Walczak-Górka

Department of Green Areas and Landscape Architecture, Poznań University of Life Sciences

Agata Walczak-Górka: agata.walczak@up.poznan.pl

The potential of greenery to mitigate the discomfort associated with road infrastructure is a significant aspect of contemporary spatial planning. With the rapid development of cities and the accompanying highways and express-ways, there is a growing need to address the negative impacts of road infrastructure on the surrounding environment. This study focuses on determining how greenery along highways and expressways can help alleviate various challenges associated with road transportation based on existing research in this area.

To thoroughly examine this topic, an extensive literature review was conducted using leading scientific databases such as Scopus and ScienceDirect. A combination of keywords was searched: ("pollution" OR "noise" OR "temperature") AND ("road" OR "highway") AND ("vegetation" OR "roadside vegetation" OR "trees"). There were 653 articles matching the specified combination of keywords (as of 7 February 2024). The analysis of this literature primarily focused on understanding the examined phytosanitary functions of roadside greenery. Despite encountering limitations such as document unavailability or incompleteness, the articles were carefully analysed to draw valuable conclusions.

The results of this study emphasize the significant role of roadside greenery in mitigating various negative effects of road traffic. Air pollution absorption, noise reduction, rainwater retention, or soil pollution reduction – greenery along transportation routes brings multifaceted benefits that contribute to improving the overall quality of the road environment and neutralizing the negative effects of road traffic.

The conclusions from the analysis provide a foundation for further discussions on sustainable urban development and the role of greenery in creating a more harmonious road environment. By combining theory and practice, the research can serve as inspiration for urban decision-makers, planners, and researchers striving to create environments around expressways and highways that are more environmentally and socially friendly.

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Keywords: greenery, roadside greenery, road discomfort, highway, expressway, environmental pollution

Optimization in Multiple Mobile Robot Systems using Multi-Agent Path Finding

Łukasz Janiec

Department of Cybernetics and Robotics, Wrocław University of Science and Technology

Łukasz Janiec: lukasz.janiec@pwr.edu.pl

My research explores the utilization of Multi-Agent Path Finding (MAPF) algorithms for optimizing time efficiency in a hybrid hierarchical multiple mobile robot system. The system architecture encompasses both high-level discrete coordination algorithm of the fleet and lower-level continuous time control of every mobile robot. The supervisor controller operates using a discrete event system. Events are generated by the continuous movement of autonomous mobile robots in a space that is discretized during system synthesis (so-called *space-as-a-resource*). Each robot requests the allocation of further resources needed to finish its task and emits resource release events. The discrete supervisor checks if the requested resources can be allocated without creating collision or first-order deadlocks with other robots. The aim is to enhance the coordination and movement of multiple mobile robots operating in complex environments by integrating offline MAPF techniques for optimized motion planning of the robots.

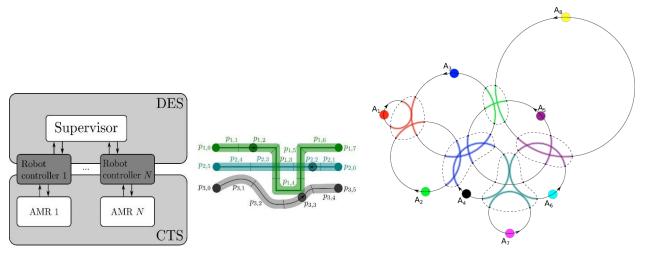


Fig. 1. Layers of control in the hybrid MMRS (left), example transportation tasks with optimized paths (middle), example cyclical paths with

Literature

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Keywords: mobile robots, discrete event system, continuous-time control, control system synthesis, multi-agent path finding

Shear strength of cement-soils doped with waste dust

Piotr Wyborski

Department of Geotechnics, Hydrotechnics, Underground and Hydraulic Engineering, Wrocław University of Science and Technology

Piotr Wyborski: piotr.wyborski@pwr.edu.pl

In order to improve the mechanical properties of the soil, chemical stabilization is a common practice [1,2]. According to [3], among many types of binders used for soil stabilization, Portland cement was considered the most effective binder with low toxicity and low cost. Currently, a very important problem is minimizing the amount of cement used, due to the significant energy input and carbon footprint generated by its production process [4].

As a sustainable approach to civil engineering, the waste resulting from aggregate processing can be used as an admixture material when producing construction materials [5]. In this study, an attempt was made to use granodiorite waste from an asphalt mixture plant as a soil-stabilizing admixture. This research presents an innovative use of granodiorite waste dust as an additive that can reduce the use of Portland cement in cement-soil mixtures while maintaining high strength parameters. In the past, researchers added mineral dust to the soil as a filler to improve the grain size and characteristics of the soil. Novelty in this study is the addition of granodiorite dust (characterized by a high silica content) to the cement-soil mixture in order to induce pozzolanic reactions to strengthen the soil material. The tested mechanical parameter of the stabilized soil was shear strength, which was determined using a direct shear apparatus. The doped soil was silt (Si). Three types of soil mixtures were tested, consisting of soil with 2% cement, soil with 4% cement, soil with 2% cement and 2% waste dust (collected from the aggregate dust cleaning system of the Ammann Asphalt precast batching plant). Four samples from each group of soil materials were tested. All samples were conditioned in a water bath for 28 days. The results showed that the addition of granodiorite dust clearly influenced the shear strength of cement soils. Samples with the addition of granodiorite dust were characterized by lower cohesion and a significantly higher value of the friction angle. A summary of the results of the shear strength test is presented in Fig. 1. The results suggest that these waste additives may be an effective method of changing the mechanical properties of cement-soils, which is of practical importance in civil engineering.

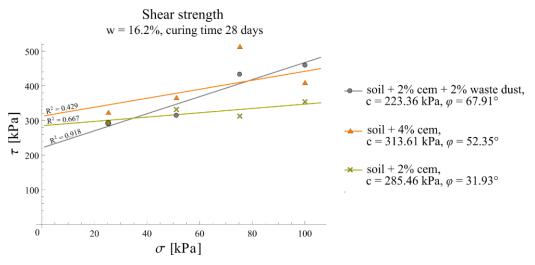


Fig. 1. Shear strength of the analyzed cement-soil mixtures

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Keywords: unsaturated soils, soil stabilization, fibers reinforcement, waste dust, granodiorite

Development of a platform for *in vivo* metabolite and neurotransmitter measurements in molecular MDD correlates

Paweł Hanus^{1, 2}

¹ Department of Psychiatry, Faculty of Medicine Wroclaw Medical University ² Biology of Astrocytes Group, Łukasiewicz Research Network – PORT Polish Center for Technology Development

Paweł Hanus: pawel.hanus@port.lukasiewicz.gov.pl

Astrocytes play a crucial role in regulating the number and functioning of synapses. Specifically, these cells are responsible for brain energy metabolism and neurotransmitter homeostasis, both processes being tightly linked at the molecular level and subject to systemic hormonal control. Disturbances in astrocyte-specific processes can lead to abnormal synaptic structure and function. For example, clinically confirmed phenotypes in depression include disrupted glucose metabolism in the prefrontal cortex and altered glutamate to glutamine (Glx) ratio. Both parameters are directly related to astrocyte function. The main glutamate metabolism pathway involves its uptake by specific transporters, activating glucose metabolism. Glutamate is then converted to glutamine (by the astrocyte-specific enzyme GluL), or it can enter the Krebs cycle as an energy substrate. Current understanding of astrocyte physiology indicates the regulation of these processes under chronic stress conditions in mice by hormones regulating circadian metabolism – glucocorticoids. The main hypothesis of the project assumes that these disturbances are the cause of abnormal neurotransmission in stress-related disorders. Monitoring circadian profiles of metabolites and major neurotransmitters with NextGenMicrodialysis will be necessary to verify the hypothesis. Translational model will be validated during measurements of changes induced by chronic stress in rodents, in brain areas integrating stress response, such as the prefrontal cortex. Study will enable identification of new molecular targets for the pharma-cotherapy of psychiatric disorders.

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Keywords: astrocytes, glucocorticoids, metabolomics, major depression disorder, translational psychiatry

Microwave filters with frequency variant couplings

Maciej Jasiński

Department of Microwave and Antenna Engineering, Gdańsk University of Technology

Maciej Jasiński: maciej.jasinski@ieee.org

From the very beginning and continuing to the present, telecommunication systems have faced the same problem: how to manage their resources to deliver service to the ever-growing number of users. One of the most common solutions is the division of the available electromagnetic spectrum into channels. Each channel has a specified spectral width – the range of signal frequencies assigned to a specific user. In such a system, all channels can be used simultaneously – the total signal in the transmission medium is a superposition of signals from each channel. Therefore, the system needs to distinguish the signal based on frequency to operate. A device – which can not only distinguish but also select the signal of a desired frequency band and reject unwanted spectral components – is called a filter. Parameters of the filter affect the entire telecommunication system - the real filter differs from the ideal one: there are transmission losses, attenuation of the out-of-band signal is finite, and there is a transition band between the passband and stopband. All these effects deteriorate the performance of the system. Therefore, to meet the very strict requirements imposed on modern telecommunication systems, designers of the filters have to seek new methods to improve their characteristics. In the field of coupled resonator filters, one of the approaches investigated by scientists and engineers is the utilization of frequency variant (dispersive) couplings in the filter structure to enhance its performance. This work provides a brief overview of such an approach undertaken by the author. The use of dispersive couplings with different profiles of frequency dependence allows the designer to modify the transmission and rejection responses of the filter. The simplest dispersive couplings - linearly or quasi-linearly variant with frequency - can introduce a transmission zero (TZ) - a frequency point at which no signal can pass through the filter. This can be used to improve the selectivity of the filter characteristic, making the transition bands narrower [1], suppressing the spurious bands, or shaping the group delay response [2] – the time it takes for a given spectral component to travel through the filter structure. For couplings described by a more complex (nonlinear) function of frequency, it is possible to produce multiple transmission zeros and even transmission poles [3] (a frequency point of full transmission). However, introducing such couplings to the filter topology complicates its mathematical description and makes the design process more challenging. Therefore, our group has established an efficient optimization-based method of filter synthesis with frequency-variant couplings. The proposed methods are validated by the design of filters with dispersive couplings, fabrication of the prototypes, and measurement. The obtained results show a high level of agreement between simulated and measured responses.

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Keywords: microwave filter, coupling matrix, frequency-variant coupling, dispersive delay structure, transmission zero (TZ)

Theoretical Studies of Photoinduced Electron Transfer in Nucleic Acids

Mikołaj Gurba, Rafał Szabla

Institute of Advanced Materials, Faculty of Chemistry, Wroclaw University of Science and Technology

Mikołaj Gurba: mikolaj.gurba@pwr.edu.pl

Photoexcitation of nucleic acid molecules by UV-vis radiation may result in the formation of damage, such as cyclobutane pyrimidine dimers (CPDs), but also in the self-repair of these damages [1]. These processes are very interesting from the point of view of research on the origin of life. Experimentally studied DNA self-repair processes use the mechanism of photoinduced electron transfer to initiate bond breaking in CPDs [2]. Many factors can influence the probability of electron transfer occurring, such as the order of the nucleotide sequence or the conformation of individual nucleotides [3]. Studying the effects of these factors on the stability of excited states can help us understand how they can be controlled by changes in nucleic acid geometry. In this study, electron transfer properties within several tri- and tetranucleotides were examined. The vertical excitation energies as well as the adiabatic excitation energies of charge transfer and locally excited S1 states were calculated using the time-dependent DFT methodology, at the CAM-B3LYP functional. To determine how the π - π stacking of adjacent nucleobases affects the energies of the charge transfer state, a novel "stacking score" calculating algorithm was developed and successfully implemented. The results suggest that the π - π stacking between nucleotide bases and the subsequent geometry of the oligonucleotide can have a strong influence on the stability of the guanine-adenine charge-transfer state.

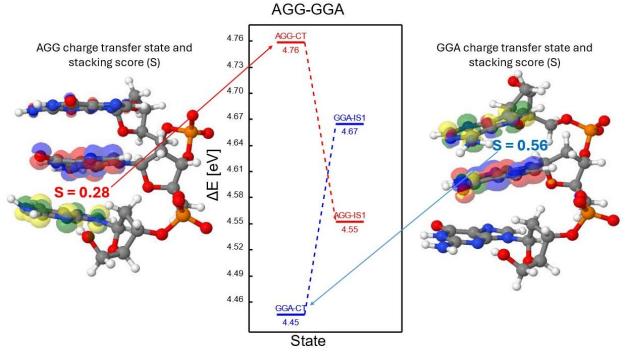


Fig. 1. The effect of nucleotide stacking on stability of charge transfer states in AGG and GGA oligonucleotides

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Keywords: quantum chemistry, photochemistry, nucleotide stacking, nucleic acids, origins of life

Single-layer Mo(S_xSe_{1-x})₂: Effect of LEDs illumination on electrical properties

Konrad Król

Department of Nanometrology, Wrocław University of Science and Technology

Konrad Król: konrad.krol@pwr.edu.pl

Two-dimensional (2D) semiconductor materials, particularly transition metal dichalcogenides (TMDs) and their alloys, have recently attracted considerable scientific and technological interest due to their unique optical and electrical properties, which are dependent on the thickness of the structure. This allows them to find a wide range of applications in optoelectronics and sensors, among others. In the present study, the electrical properties of monolayer structures based on $Mo(S_xSe_{1-x})_2$ crystals were investigated. The samples were prepared using mechanical exfoliation and the dry transfer method [1]. To characterize the number of layers, Raman spectroscopy measurements were performed, which prove that single crystal layers were obtained. Specially prepared SiO₂/Si substrates with 5 μ m separated gold planar electrical contacts were used to fabricate the structures (Fig. 1a). The electrical properties of devices, including 2D semiconductors, depend on temperature. In the case of $MoS_{0.5}Se_{1.5}$, with increasing temperature, the observed resistance changed nonlinearly – it decreased from 40 M Ω at T = 80 K to 630 k Ω at T = 450 K. In addition, I investigated the effect of illuminating the sample with LEDs of different wavelengths on the electrical properties of $MoS_{0.5}Se_{1.5}$ based structures (Fig. 1b). This material shows the best properties when exposed to light with a wavelength (λ LED) of 630 nm and around 250 K, at which the highest photocurrent is generated (i.e., 390 nA), while the worst properties occur around T = 150 K and at the same time 10 times lower. In the case of other Mo(S_x Se_{1-x})₂ alloys, the best properties were observed at a higher temperature, i.e., around T = 300 K. Furthermore, at similar temperatures, the wavelength of the illumination used also matters. The largest effect on photocurrent is noticed for illumination with a wavelength of 630 nm, while the smallest – for $T < 290 \text{ K} - \lambda \text{LED} = 519 \text{ nm}$. The results presented here show that $Mo(S_xSe_{1-x})_2$ alloy-based devices can function as temperature sensors or photodetectors.

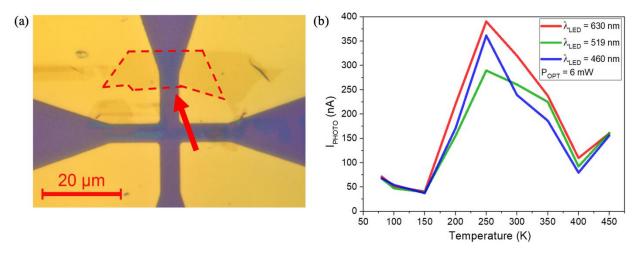


Fig. 1. (a) The single atomic layer of MoS_{0.5}Se_{1.5} alloy on a specially prepared silicon substrate covered with SiO₂ layer and gold contacts; (b) Effect of temperature (*T*) and LEDs illumination with wavelengths (λ LED) of 460 nm, 519 nm and 630 nm and optical power (*P*_{opt}) of 6 mW on the photocurrent (*I*_{photo}) of the MoS_{0.5}Se_{1.5} alloy monolayer

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Keywords: transition metal dichalcogenides (TMDs), 2D materials, electrical properties, photodetector, electrical measurements

Interactions of fructose 1,6-bisphosphatase forms with hypoxia-inducible factor 1a

Bartosz Budziak¹, Piotr Hinc¹, Dariusz Rakus¹, Aleksander Czogalla²

¹ Department of Molecular Physiology and Neurobiology, University of Wrocław ² Department of Cytobiochemistry, University of Wrocław

parament of Cytoblochemistry, emitersity of whee

Bartosz Budziak: bartosz.budziak@uwr.edu.pl

In cancer cells, the presence of hypoxia-inducible factor 1α (HIF1 α), a master regulator of the transcriptional response to hypoxic conditions, can be affected in a non-enzymatic manner by fructose 1,6-bisphosphatase (FBP) [1]. Both isozymes of FBP, namely liver (FBP1) and muscle (FBP2) forms are potential interaction partners with HIF1 α . Those isozymes have two main conformations: active R-state (relaxed) and, after allosteric inhibition, inactive T-state (tense), with different parts of the protein surface available for protein-protein interactions [2].

Quantitative data on the interaction of FBP1 and FBP2 with HIF1 α *in vitro*, in the presence and absence of natural and synthetic allosteric effectors of FBP shows differences between FBP isozymes. FBP1 interacts with HIF1 α with similar dissociation constants in both T and R states, while FBP2 affinity to HIF1 α is strongly dependent on its conformation. The dynamic regulation of FBP2-HIF1 α complex formation is strong evidence that this isozyme has a bigger role in maintaining HIF1 α levels in cells than FBP1. The difference is probably caused by distinct conformational changes in FBP oligomers in response to the allosteric effectors [2].

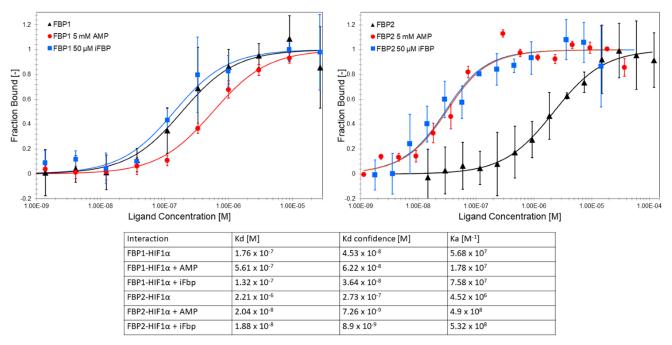


Fig. 1. Quantitative interactions of different forms of FBP with HIF1 α

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Keywords: fructose 1,6-bisphosphatase; binding constants; cancer; hypoxia; moonlighting proteins

Syngas from waste biomass

Alina Krokoszyńska, Piotr Rutkowski

Department of Process Engineering and Technology of Polymer and Carbon Materials, Wrocław University of Science and Technology, Faculty of Chemistry, 7/9 Gdańska Street, 50-344 Wrocław

Alina Krokoszyńska e-mail: alina.krokoszynska@pwr.edu.pl

The acquisition of new green energy solutions in the chemical and energy industry sectors has been one of the main trends in recent years. Renewable energy sources such as wind, solar and hydropower, geothermal and biomass are complemented by new technological solutions. Waste biomass, the global amount of which is still growing, is a very attractive material in terms of energy. Obtained from farms, residues from gardening, as well as industrial and municipal waste, properly managed it is widely used in the production of electricity and heat. The importance of biomass in the renewable energy sector is constantly increasing. The PhD thesis in the field of chemical engineering aims to design and optimize the process of obtaining syngas through of gasification. Gasification of biomass is a series of thermochemical transformations taking place at an elevated temperature between the organic part of a coal substance and a gasifying factor, such as oxygen, water vapour, air, or carbon dioxide. The aim of the process is to produce gaseous fuel – syngas, which is widely used in industry. The energy properties of the obtained gas are primarily influenced by the type of gasification factor used and process parameters such as temperature and pressure [1]. The technology of gasification of bio-waste, purification of gas before combustion and combustion in optimal, stable conditions appears to be an acceptable and preferred technology for the coming years.

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Keywords: waste biomass, syngas, hydrogen, plasma gasification

Stoppin permeation: sol-gel coatings as a response to hydrogen-induced challenges

Natalia Kaczmarczyk, Jerzy Detyna, Justyna Krzak

Department of Mechanics, Wrocław University of Science and Technology, Smoluchowskiego 25, 50-370 Wrocław, Poland

Natalia Kaczmarczyk: natalia.kaczmarczyk@pwr.edu.pl

As global energy consumption continues to increase, the need for alternative energy sources is increasing due to the adverse environmental impact of conventional energy sources such as coal, oil and gas. Hydrogen is emerging as a promising solution. Its appeal lies in its abundance, versatility, and most importantly, its potential to produce energy without emitting harmful pollutants or greenhouse gases [1]. However, challenges arise from its properties, including low density and high mobility, which result in high permeability and difficulties in storage or transport, especially through polymeric materials used in high-pressure tanks. To address these challenges, efforts are focused on improving tank integrity, with the dominant method being the application of coatings inside composite high-pressure tanks, made with composite and polymeric linear [2]. This study explored the potential of sol-gel coatings made of silicon oxide or aluminum oxide as effective barriers against hydrogen penetration in polymer substrates. Sol-gel coatings offer advantages such as tunable properties, environmentally friendly synthesis, and compatibility with polymer substrates [3]. This research is aimed at understanding the properties and applications of sol-gel coatings in order to significantly improve the tightness of type IV high-pressure tanks. Such advances will improve the safety and efficiency of hydrogen storage systems, meeting a key need in the transition to sustainable energy solutions.

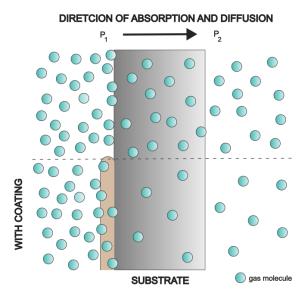


Fig. 1. Hydrogen permeation through substrate and substrate with barrier coating

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Keywords: hydrogen permeation, sol-gel coating, barrier properties

Atomization of metal powders in high-power ultrasonic field

Adam Sajbura, Paweł Sokołowski

Department of Metal Forming, Welding and Metrology, Faculty of Mechanical Engineering, Wrocław University of Science and Technology

Adam Sajbura: adam.sajbura@pwr.edu.pl

Currently, there is huge interest in metal and metal alloy powders on the market. The main reason causing development in that field is the wide-scale spread of additive manufacturing and coating applications. Modern production technologies require powders with, e.g., highly spherical shape, dedicated particle size and narrow particle size distribution. Failure to meet these requirements involves, among others, with significantly poorer surface quality of the obtained details, the possibility of occurrence of inclusions of unmelted material or increased porosity of the elements.

Metal powder production involves various methods such as atomization, chemical reduction, and mechanical comminution, each tailored to produce fine particles of metals with specific properties. Atomization uses energy delivered by high-pressure gas or liquid, ultrasonic waves, or plasma to break molten metal into droplets that solidify into powder. The most common methods are gas atomization and water atomization. Powders produced by this method of production serve as crucial raw materials for additive manufacturing, powder metallurgy, and other advanced applications in industries ranging from aerospace to automotive.

In this work, ultrasonic atomization is proposed as an alternative route for powder materials manufacturing. When compared to gas or water atomization, it requires a smaller chamber due to the narrower spread of the sprayed material in the process. Reducing the working chamber brings many benefits, such as:

- possibility of producing small batches of material for research and development purposes;
- reducing the amount of gas necessary to flush the chamber and speeding up the process;
- possibility of carrying out the process in laboratory conditions without the need to have large-scale industrial facilities.

An important factor in favor of the development of ultrasonic atomization technology is also the fact that the powder size distribution can be controlled using the vibration frequency of the atomization tool, i.e., it is concluded that the higher the vibration frequency, the finer material will be. The melting parameters of the material also have a significant impact on the process of producing powders using ultrasonic atomization, as it is necessary to introduce the material into a liquid state. Therefore, an important parameter will be the distance between the material melting system and atomization unit.

The work discusses the ultrasonic atomization technology demonstrator. The atomization trials confirmed the ultrasonic atomization capacity to produce powder with controllable size and narrow distribution. Furthermore, the obtained powder was defect-free and nearly spherical, which is the clue for its further usability. The influence of relative position of the melting system and the atomization unit was examined too. The results show both the stability of the process and the possibility of interference in the characteristics of the obtained materials.



Fig. 1. Ultrasonic atomization technology demonstrator

Keywords: metal powders, ultrasonic atomization, additive manufacturing, thermal spraying

Hexadecane biodegradation by electroactive consortia in microbial fuel cells

Natalia Tyszkiewicz^{1, 2}, Piotr Młynarz², Grzegorz Pasternak¹

¹ Laboratory of Microbial Electrochemical Systems, Faculty of Chemistry, Wrocław University of Science and Technology,

Wyb. Wyspiańskiego 27, 50-370 Wrocław, Poland

² Department of Biochemistry, Molecular Biology and Biotechnology, Faculty of Chemistry,

Wrocław University of Science and Technology, Wyb. Wyspiańskiego 27, 50-370 Wrocław, Poland

Natalia Tyszkiewicz: natalia.tyszkiewicz@pwr.edu.pl

Hexadecane, a component of petroleum hydrocarbons, poses a serious environmental hazard due to its widespread occurrence as a contaminant in soil and water systems. Its persistence and resistance to degradation require innovative remediation strategies. Microbial fuel cells (MFCs) represent a promising approach to bioremediation that uses the metabolic activity of microorganisms to degrade pollutants while generating electricity. One of the pathways for hexadecane degradation involves biosurfactant-assisted degradation, where microorganisms produce biosurfactants independently or through cooperative interactions, enhancing the solubilisation and bioavailability of hydrophobic compounds like hexadecane. In this study, we investigate the biodegradation of hexadecane using electroactive consortia in MFCs to elucidate their respective capabilities and potential synergistic effects in enhancing remediation efficiency, biosurfactant production, and power generation.

For this purpose, 24 single-chamber MFCs were designed and constructed. The MFCs were inoculated with 1) mixed consortium enriched in MFCs fed with crude oil, 2) synthetic consortium of *Pseudomonas aeruginosa*, *Serratia marcescens*, and *Rhodococcus erythropolis*, 3) mixed consortium of soil from Sri Lanka enriched in MFCs and 4) activated sludge from a wastewater treatment plant. The anode chambers were filled with minimal salt medium (MSM) with hexadecane (1.23 mM) and acetate (12.2 mM) as carbon sources. The growth dynamics of microorganisms was observed by real-time voltage monitoring and LSV, CV and EIS measurements of MFC. GC-MS and COD analysis was carried out to assess the removal rate of hexadecane. For biosurfactant extraction, liquid extraction with ethyl acetate was used.

As a result, the highest generated power of 125.61 μ W (139.57 mW/m²) was obtained for activated sludge as an inoculum. MFCs operating in a mixture of different microbial strains exhibit greater power output due to metabolic synergy, enhanced metabolic diversity, and increased resistance to environmental variations. COD analysis showed that both acetate and hexadecane were degraded in MFC to a significant degree. Moreover, GC-MS analysis showed almost 99% degradation of hexadecane at the end of the cycle in MFCs on activated sludge. Samples after biosurfactant extraction showed significant decreases in surface tension to a value of about 45 mN/m, indicating the production of surfactant compounds during hexadecane degradation. These results highlight the potential of MFC technology as a sustainable and environmentally friendly approach to removing pollutants such as hexadecane from the environment. In the future, 16S rRNA analysis will be required to identify key strains in the most effective MFCs. Analysis of the obtained biosurfactants is ongoing. On the basis of the results obtained, activated sludge was selected as the best inoculum and will be used in future steps for an experiment to track the metabolic pathways of bioelectrochemically assisted biotransformation.

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Keywords: hexadecane, biodegradation, MFC, electroactive consortia, biosurfactants

Bioelectrochemical stimulation of biodegradation of petroleum products in bioelectrochemical systems

Bartosz Widera, Piotr Rutkowski, Grzegorz Pasternak

Department of Process Engineering and Technology of Polymer and Carbon Materials, Faculty of Chemistry, Wrocław University of Science and Technology, 50-370 Wrocław, Poland

Bartosz Widera: bartosz.widera@pwr.edu.pl

Bioelectrochemical systems (BES) represent an innovative approach in the field of chemical engineering. These systems exploit the properties of electroactive microorganisms to carry out oxidation reactions of organic compounds [1]. The product of these chemical transformations is mainly electrical energy, which can be used to power other devices. One of the most classical examples of BES is the Microbial Fuel Cell (MFC). In this configuration, microorganisms engage in an oxidation reaction of organic matter on the anode electrode, resulting in the production of protons and electrons. These products are then used for further reduction reactions that take place at the cathode. Figure 1 illustrates the basic configuration of MFCs, comprising a single- or two-chamber cell [1]. The undoubted advantages of these systems are their gentle mode of operation, and the possibility of using a wide range of compounds as a carbon source, including petroleum-based compounds.

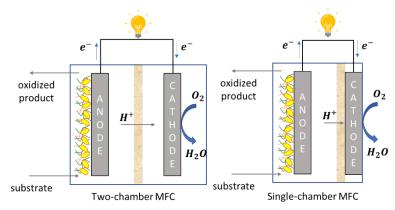


Fig. 1. Schematic of Microbial Fuel Cells

Petroleum compounds, including aliphatic, acyclic, and aromatic hydrocarbons, are common environmental pollutants. These substances can adversely affect the functioning of plants, animals, and humans. Particularly dangerous are the compounds of BTX (benzene, toluene, and the three xylene isomers), the concentrations of which in the environment are strictly regulated [2]. These compounds can be successfully degraded in BES, making these systems a good alternative to classical remediation methods [3, 4]. Furthermore, processes in bioelectrochemical systems can lead to the production of beneficial chemicals, such as biosurfactants. These compounds are used in various industries, including the production of cleaning products and cosmetics. Furthermore, biosurfactants have been shown to have a positive effect on BES performance by accelerating cell start time, increasing energy production, or improving organic matter bioavailability [5].

Bioelectrochemical systems represent a promising technology in chemical engineering that can contribute to the reduction of petroleum-based pollutants by effectively using the activity of electroactive microorganisms. The application of this technology has the potential to improve environmental quality, facilitate the use of renewable energy sources, and produce valuable chemical compounds.

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Keywords: bioelectrochemical systems, electroactive microorganisms, petroleum products, biodegradation, electrochemistry

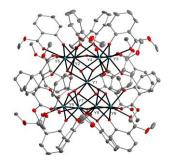
Sandglass-like nonanuclear rare-earth molecular cluster aggregates for alkaline-earth manganite oxide nanomaterials doping

Adrian Kowaliński, Rafał Petrus

Department of Biochemistry, Molecular Biology and Biotechnology, Faculty of Chemistry, Wrocław University of Science and Technology, Smoluchowskiego 23, 50-370 Wrocław

Adrian Kowaliński: adrian.kowalinski@pwr.edu.pl

Over the past few decades, lanthanide molecular cluster aggregates (MCAs) composed of multinuclear metal core encapsulated by organic ligands have garnered much attention because of their interesting solid-state structures and versatile application in the field of single molecular magnetism [1], magnetic refrigeration systems [2], luminescent sensors/probes [3], and catalysis [4]. Recently, MCAs are being considered as the new generation of highly efficient optical materials that can unify the properties of lanthanide nanoparticles (NPs) and molecular complexes. Because of the chemical similarities of Ln(III) ions, the easy modification of the chemical composition and, consequently, the energy transfer processes using MCAs are similar to those observed for NPs. The molecular architecture of the lanthanide clusters allows for a precise determination of the Ln(III) local symmetry, leading to higher homogeneity in the optical properties, which is not entirely possible for NPs. Lanthanide complexes can also be used as molecular precursors for the low-temperature synthesis of functional organic materials [5].



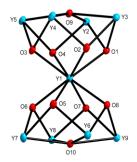


Fig. 1. The molecular structure of $[Y_9(\mu_4-OH)_2(\mu_3-OH)_8(L)_{16}]$ Cl. The displacement ellipsoids are drawn at the 10% (a) or 20% (b) probability level. Hydrogen atoms and disorder counterparts of aromatic ligands are omitted for clarity

Because of that, we decided to use nonanuclear $[RE_9(\mu_4-OH)_2(\mu_3-OH)_8(L)_{16}]^+$ clusters (RE = Y, Eu, Dy, Tm, Yb, Lu; L = methyl or ethyl salicylate) pictured in Figure 1 as a single-source of rare-earth ions for doping bimetallic oxide nanomaterials (CaMnO₃ and BaMnO₃) obtained from thermal decomposition of manganese $[Mn_2(\mu-OMe)_2(L)_4]$ and calcium $[Ca(L)_2]n$ or barium $[Ba(L)_2(THF)]_n$ clusters, as shown in Figure 2. The research conducted proved that:

- a. thermal decomposition of manganese and calcium compounds together with rare-earth metal complexes led to the formation of $CaMnO_3$ as the main phase and small amounts of $CaMn_2O_4$ doped with RE^{3+} ions;
- b. thermal decomposition of manganese and barium compounds together with rare-earth metal complexes led to the formation of $BaMnO_3$ doped with RE^{3+} ions;
- c. REMnO $_3$ crystallites are present in the BaMnO $_3$:RE materials.

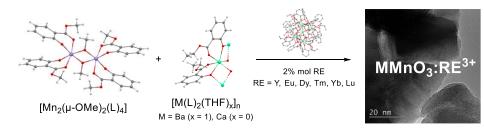


Fig. 2. Thermal decomposition of complexes to $MMnO_3:RE^{3+}$ (M = Ba, Ca)

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Keywords: rare-earth metals, heterometallic compounds, molecular precursors, molecular cluster aggregates

Carbon-Based OER Electrocatalysts: Paving the Way for Green Energy Transformation

Izabela Walendzik, Karolina Kordek-Khalil, Piotr Rutkowski

Department of Process Engineering and Technology of Polymer and Carbon Materials, Wrocław University of Science and Technology

Izabela Walendzik: izabela.walendzik@pwr.edu.pl

The growth of the world's population leads to an increasing demand for energy. Shrinking fossil fuel resources and the development of renewable energy sources require the transformation of efficient energy storage and conversion technologies. Hydrogen emerges as an attractive energy carrier not only due to its high gravimetric energy density and zero CO_2 emissions, but also because of the promising green method of its production – water electrolysis.

The advancement of ubiquitous electrical devices entails increasing user demands for performance and durability. Zinc-air batteries may present a promising alternative to lithium-ion batteries due to their low cost, safety, and environmental friendliness.

However, both technologies require an improvement in the oxygen evolution reaction (OER), whose slow kinetics diminishes device efficiency. The solution may lie in the use of a suitable electrocatalyst. Proper electrode material can lower the energy required for the reaction to take place and consequently improve performance of the device.

A promising group of materials for addressing this challenge are carbon materials, particularly nanostructures such as carbon nanofibers and nanotubes. An attractive perspective in the use of carbon materials for electrocatalytic purposes is also the application of inexpensive, flexible, and conductive carbon cloth as a substrate for the synthesis of carbon nanostructures. This approach enables the development of a freestanding electrocatalyst, which can be successfully used as a high-performance electrode material in a model water electrolyzer or Zn-air battery.

The research was funded by the Empiria i Wiedza Foundation under the research project "Talenty Jutra".

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Keywords: carbon materials, electrocatalysis, oxygen evolution reaction, Zn-air batteries, water electrolysis

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Using ionic surfactant mixtures as a promising approach to designing novel flotation chemistry collector systems

Krzysztof Jan Legawiec, Mateusz Kruszelnicki, Izabela Polowczyk

Department of Process Engineering and Technology of Polymer and Carbon Materials, Wrocław University of Science and Technology

Krzysztof Jan Legawiec: krzysztof.legawiec@pwr.edu.pl

Flotation is a process of selective separation of solid particles dispersed in a liquid by using air bubbles. This process is carried out in a device where finely milled mineral ore is dispersed in water. Gas bubbles introduced into this mixture selectively attach to the ore particles, lifting them to the surface, where they form a froth layer that is collected as the product of the process. Flotation is employed across various sectors, including wastewater management, plastic recycling, and paper purification, but it is predominantly utilized in mineral ore processing to separate valuable minerals from waste minerals.

A crucial aspect of the flotation process is the attachment of desired mineral particles to air bubbles. To achieve selective separation of ore components using bubbles, different chemical agents are employed to modify the surface characteristics of the particles effectively. A crucial role is played here by reagents known as collectors – they have the ability to adsorb on the surface of the target minerals, increasing their hydrophobicity. Surface-active substances such as anionic and cationic surfactants may successfully act as a collector. Recent research shows that using a combination of both anionic and cationic surfactants can significantly enhance the flotation process efficiency. This approach helps optimize the process performance and selectivity. However, many studies tend to focus solely on the process outcomes without addressing the fundamental mechanisms of how particles attach to bubbles.

Our work concentrates on examining the interactions between gas bubbles and mineral surfaces in presence of mixed surfactant system. To achieve this, we employ an adhesion dynamics test system that enables us to observe these processes, which often last only milliseconds. The experimental results involving mixtures of anionic and cationic surfactants provide data that will be verified in future flotation experiments. This will enable us to extend the fundamental research results of to fully exploit the application potential of the proposed technological separation approach, thereby facilitating the selection of the most promising solutions.

This work was supported by the National Science Centre, Poland (project number 2023/49/N/ST8/04259, Surfactant synergy in flotation process: Exploring the impact of anionic/cationic surfactants mixtures on thin liquid film stability.

Keywords: flotation, three-phase contact, anionic surfactant, cationic surfactant

Hybrid adaptive controllers applied to electric drives with flexible links

Radosław Stanisławski, Marcin Kamiński

Department of Electric Machines, Drives, and Measurements, Wrocław University of Science and Technology

Radosław Stanisławski: radoslaw.stanislawski@pwr.edu.pl

Modern electric drives need to be designed to fulfill strict response demands. The desired speed and position must be followed with minimal latency and overshoot. In most cases, an ideally stiff connection between the motor and the load machine is assumed, which greatly simplifies the controller design process. However, in applications such as robotic manipulators [1], wind turbines [2], exoskeletons [3], and electric cars [4], if the flexibility of the connecting elements is not taken into account, oscillations of speed and torsional torque may impair the operation of the drive. Amongst many, the following disadvantages can be listed: deterioration of the drive's mechanical parts, difficulty with controlling the state variables, and even possible stability loss [5].

Methods used to deal with oscillations of state variables can be divided into passive and active solutions. Passive approach focuses on mounting mechanical dampeners [6]. However, in this case not only the cost of the drive is increased, but also its reliability is reduced (additional elements become another possible source of failure). Active techniques rely on establishing a control signal for the electric motor that will not cause the oscillations to appear. One of the most often implemented controllers is the PID controller [7]. However, it is not capable of providing adequate control signals as it does not include information about the state of the load machine. Its performance can be improved by supplying additional feedback from other state variables [8], or by substituting the PID controller with a State Feedback Controller (SFC) [9]. Still, both of these solutions are very sensitive to plant parameter changes. Usually these controllers are tuned using the root locus method, which requires the plant parameters to be known. If the parameters are not correctly identified or change during the operation of the drive (e.g., increase in load inertia), the controller's gains will be set inadequately, resulting in a hindered drive response. Therefore, adaptive control schemes need to be investigated.

The research is focused on enhancing classic methods (such as PI or SFC) by incorporating a Radial Basis Function Neural Network (RBFNN) into the control structure. RBFNNs are usually applied as adjustment mechanisms for the gains, so that the controller remains correctly tuned [10]. In the performed studies, however, RBFNN is added as an independent tool. Its training is performed during the drive's operation, meaning it can learn proper drive behavior and respond to sudden changes in plant parameters, providing a correction signal for the original structure (hence the hybrid nature of the proposed controllers). Examples of the obtained results can be seen in [11, 12].

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Keywords: electric drives, flexible links, control theory, adaptive control, radial basis function neural networks

Biological and physical pretreatment of spent hops enhances extraction of xanthohumol

Aleksandra Modzelewska, Anna Trusek, Mateusz Jackowski

Department of Micro, Nano and Bioprocess Engineering, Faculty of Chemistry, Wrocław University of Science and Technology

Aleksandra Modzelewska: aleksandra.modzelewska@pwr.edu.pl

Pretreatment of plant biomass samples prior to further processing steps, when performed successfully, can lead to a higher yield of the overall process. Biomass can be treated in a variety of methods, including biological, chemical or physical pretreatment, or by applying a combination of them. Physical methods include microwave-assisted extraction, ultrasound-assisted extraction or pressurized liquid extraction [1], while biological pretreatment methods use, i.e., cell wall degrading enzymes [2].

Spent hops from supercritical hop extract production (Fig. 1) are a rich source of valuable compounds. One of them is xanthohumol (Fig. 2), a prenylated flavonoid in the hop plant flower, which was proven to have antiviral, antibacterial, anti-inflammatory and anti-cancerogenic properties [3]. Conditions under which supercritical extraction takes place do not change the concentration of xanthohumol in the biomass, as its solubility in $scCO_2$ is particularly low, therefore the by-product from this process can be a rich source of this substance.



Fig. 1. Spent hops from a supercritical extraction plant

This research focuses on the extraction of xanthohumol from spent hops obtained from a supercritical extraction plant (Puławy, Poland). A variety of pretreatment methods are used, including microwaves, ultrasounds, freeze-thaw, as well as the use of enzymes (cellulase blends). The preliminary experiments so far show promising results, as, for example, the use of microwaves in spent hops allows for an increase in extraction of xanthohumol by approximately 20% compared to samples that have not been pre-treated.

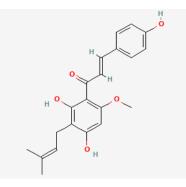


Fig. 2. Xanthohumol

The work was supported by the Minigrants project for doctoral students of the Wroclaw University of Science and Technology.

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Keywords: spent hops, biomass pretreatment, extraction, xanthohumol

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