Book of Abstracts

Saxony meets Lower Silesia:

Science across Borders

Conference

Dresden

17.-18 June 2024

Contents

Committees

General Chairs

Prof. Dr. Dr. hc. mult. Sebastian M. Schmidt, Scientific Director, HZDR, Germany

Prof. Dr. hab. Robert Olkiewicz, Rector of the University of Wroclaw, Poland

Local Organizing Chairs

Prof. Dr. Thomas D. Kühne, CASUS, HZDR, Germany

Prof. Dr. hab. Eugeniusz Zych, University of Wroclaw, Poland

Dr.PD. Agnieszka Kuc, CASUS, HZDR, Germany

Prof. Dr hab. Dr h.c. mult. David Blaschke, University of Wroclaw, Poland

Dr. Martin Laqua, Public Relation, CASUS, HZDR, Germany

Weronika Mazur, International Collaboration and Research Funding, CASUS, HZDR, Germany

Michal Bajda, Event Management, CASUS, HZDR, Germany

Rafael Koprowski, Content Development and Marketing, CASUS, HZDR, Germany

Scientific Committee

Prof. Dr. Thomas D. Kühne, CASUS Funding Director, HZDR, Germany

Prof. Dr. Karim Fahmy, Biophysics, HZDR, Germany

Prof. Dr. Ralf Schützhold, Theoretical Physics, HZDR, Germany

PD Dr. Agnieszka Kuc, Theoretical Chemistry, CASUS, HZDR, Germany

Dr. Katrin Pollmann, Biotechnology, HZDR, Germany

Dr. Franziska Lederer, Leader of the HZDR Junior Research Group BioKollekt, HZDR, Germany

Dr. Sandra Hamann, Strategy and Programs, HZDR, Germany

Prof. Dr. hab. Eugeniusz Zych, Chemistry, University of Wroclaw, Poland

Prof. Dr hab. Dr h.c. mult. David Blaschke, Theoretical Physics, University of Wroclaw, Poland

Prof. Dr. hab. Aleksander Czogalla, Biotechnology, University of Wroclaw, Poland

Prof. Dr. hab. Dorota Nowak, Biotechnology, University of Wroclaw, Poland

Dr. Justyna Zeler, Chemistry, University of Wroclaw, Poland

Program

Monday, 17.06.2024

09:30-10:30	**Arrival & Registration**		
10:30-10:45	**Opening S. M. Schmidt & R. Olkiewicz**		
10:45-11:45	**AI & Simulation, Big Data & Analytics**		
	Invited Talk	Mariusz Ptak	Numerical Models of Human Brain and the Development of Machine Learning Algorithms to Analyse Weather Conditions for the Prediction of Cerebrovascular Accidents
	Pitch	Krzysztof Graczyk	Deep learning in Monte Carlo simulation of neutrino-matter interactions and studies of porous media properties
	Pitch	Sebastian Makuch	Simulation of GNSS LEO satellites constellation for 3D water vapor monitoring
11:45-12:00	Coffee Break		
12:00-13:15	Invited Talk	Michael Bussmann	Will data help us to address future challenges?
	Pitch	Artur Yakimovich	Novel Machine Learning Approaches to Study Infection and Disease through Biomedical Images
	Pitch	Bartosz Brzoza	SE(3)-Transformers for predicting the electronic structure of hydrogen molecules
	Pitch	Ricardo Martínez - García	Dryland conservation as an interdisciplinary problem, or how to combine big data, simulation and mathematical models, and simple experiments to support ecosystem management
13:15-14:15	Lunch		
14:15-16:00	**Sustainability & Circular Economy**		
	Invited Talk	Anna Potysz	Addressing the scientific aspects of a circular economy: insight into secondary resource management
	Pitch	Milad Eftekhari	Effect of Ultrafine Particles on Film Stability and Particle Attachment
	Pitch	Nora Schönberger	Next-Gen Biosorbents: Peptides for Resource Recovery
	Pitch	Ashak Mahmud Parvez	Assessment of recyclability of modern printed circuit boards (PCBs) from technical, sustainability and economic perspectives
	Pitch	Mateusz Kruszelnicki	Sustainable flotation solutions: Investigating the impact of biological origin surfactants on bubble-particle interactions
	Pitch	Krzysztof Legawiec	Development of functionalized cellulose nanostructures for controlled and efficient aggregation of fine mineral particles towards sustainable mineral engineering
16:00-16:10	Conference Photo		
16:10-16:30	Coffee Break		
16:30-18:00	**Walk and Talk in Dresden**		
18:30-	**Get Together & Conference Dinner**		

Tuesday, 18.06.2024

09:00-10:45	**Novel Materials**		
	Invited Talk	Rico Friedrich	Data-driven Design of Novel Ionic Two-dimensional and High-entropy Materials
	Pitch	Agnieszka Kuc	Novel two-dimensional materials for applications in chemistry, physics, and materials science
	Pitch	Joanna Grzyb	Nanomaterials - a platform or a cargo in a delivery into a living cell
	Pitch	Justyna Zeler	Exploring Thermoluminescence and Luminescence Thermometry Processes in Phosphors
	Pitch	Eugeniusz Zych	When Luminescence Thermometry Can Compete with Pyrometry?
	Pitch	Hossein Tahmasbi	An Automated Materials Discovery Approach with Machine Learning
10:45-11:15	Coffee Break		
11:15-12:00	**Poster Session**		
12:00-13:00	Lunch		
13:00-14:45	**Digital Health & Life Sciences**		
	Invited Talk	Elżbieta Gumienna-Kontecka	Harnessing the power of microbial siderophores for nuclear imaging
	Pitch	Ellen Adams	Cation Specific Stabilization of FUS Biomolecular Condensates
	Pitch	David Pape	METABOLATOR: Establishing a Citable Web Application for Automated Metabolic Load Analysis
	Pitch	Xinne Zhao	Droplet-Based Microfluidics for Point-of-Care Monitoring of Biomarker Levels in Clinical Diagnostics
	Pitch	Zeljko Janicijevic	Multiplexed Extended-Gate Field-Effect Transistor Biosensing Systems: Powerful and Cost-Effective Tools for the Future of Digital Healthcare
	Pitch	Olga Michel	Anti-SARS-CoV-2 platform based on maleimide-functionalized liposomes
14:45-15:15	Coffee Break		
15:15-16:00	**Closing session: Summary & General Discussion about Future Cooperations & Projects**		

AI & Simulations + Big Data Analytics

Invited Talk - Mariusz Ptak

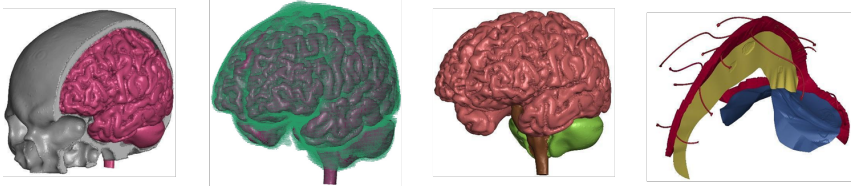
Numerical Models of Human Brain and the Development of Machine Learning Algorithms to Analyse Weather Conditions for the Prediction of Cerebrovascular Accidents

Mariusz Ptak[1]

[1] *Wrocław University of Science and Technology, Wrocław, Poland*

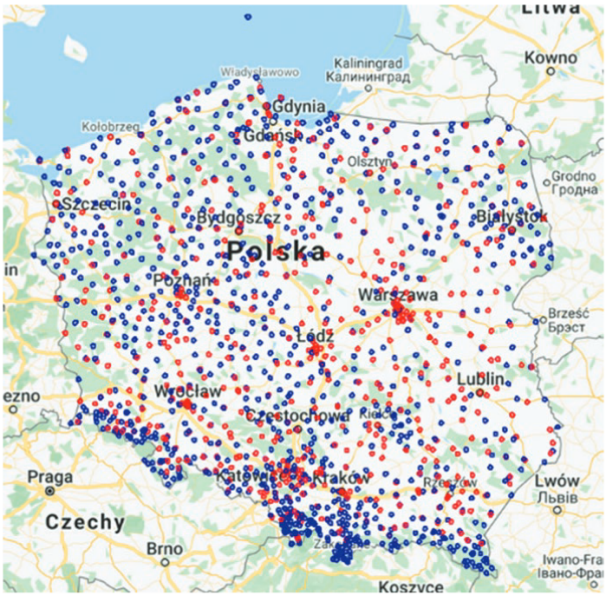
mariusz.ptak@pwr.edu.pl

Understanding the pathomechanism behind brain structure destruction is crucial for effective prevention and treatment strategies. The aHEAD project addresses this by continually enhancing diagnostic techniques and simulating the impact on brain structures resulting from road accidents, sports injuries, and head protection device efficacy, such as ski, bicycle, and motorcycle helmets. Through collaboration with neurosurgeons and neurobiologists, the project synthesizes extensive knowledge of brain structure properties and utilizes experimental studies to obtain precise input data for numerical head models. This interdisciplinary endeavor integrates medical imaging processing, advanced material processing, biomechanics, computer science, and neurosurgery to develop state-of-the-art models representing different age groups. Following rigorous validation, numerical brain tissue structural destruction simulations under mechanical loading are achieved using LS-DYNA and Abaqus codes. These simulations enable a deeper understanding of injury mechanisms and facilitate the refinement of protective measures.



In parallel, a study investigates the influence of environmental conditions on vascular incidents, aiming to develop a predictive model. Interestingly, the aHEAD models feature advanced cerebrovascular systems (such as pressured bridging veins), which enabled the authors to verify some research hypotheses connected with weather conditions. Leveraging machine learning algorithms and medical data, a recursive neural network architecture is tailored to analyze weather-related risk factors for vascular events across different diagnostic groups. Results suggest a significant association between environmental conditions and vascular incidents, particularly for spontaneous hemorrhages. Despite challenges such as incomplete medical data, the developed model demonstrates promising predictive capabilities, offering insights for enhanced patient care and hospital preparedness. Future efforts will focus on obtaining more comprehensive data and refining anomaly detection methods to improve model accuracy and applicability. These initiatives underline the

importance of interdisciplinary collaboration and advanced technological solutions in advancing medical research, diagnosis, and patient care.



References:

1. 10.1007/978-3-031-34884-6_16
2. 10.1007/s43452-023-00758-9

Acknowledgement of financial support: I extend my gratitude to the dedicated members of the aHEAD project team whose expertise and collaborative efforts have been instrumental in the success of this research endeavor.

Pitch Talk - Krzysztof Graczyk

Deep learning in Monte Carlo simulation of neutrino-matter interactions and studies of porous media properties

Krzysztof Graczyk[1]

[1] *University of Wrocław, Wrocław, Poland*

krzysztof.graczyk@uwr.edu.pl

Deep learning (DL) techniques have become a crucial tool in various areas of physics, assisting in the acceleration and optimization of computational systems. DL algorithms enable the discovery of new relations and phenomenological laws. In my presentation, I will discuss two physics problems our team is working on. Firstly, we aim to develop an AI-supported version of NuWro, a Monte Carlo generator of events used to simulate neutrino interactions with atomic nuclei in the energy range typical for long and short-base line oscillation experiments. Secondly, we will discuss our work on developing DL techniques to study fluid flow and diffusion properties in porous materials. My talk is based on three publications [1-3].

References:

1. arxiv:2312.17298
2. arxiv:2308.13222
3. Sci. Rep. 13, 9769 (2023).

Acknowledgement of financial support:

Pitch Talk - Sebastian Makuch

Simulation of GNSS LEO satellites constellation for 3D water vapor monitoring/Buss

Sebastian Makuch[1]

[1] *University of Wrocław, Wrocław, Poland*

120945@student.upwr.edu.pl

The GNSS signal is an important data source for weather applications: ground-based stations produce point-like observations of water vapor with unprecedented stability and a fast update rate. Space-based receivers mounted on the LEO satellites deliver reliable profiles of the troposphere, regardless of weather conditions. Both data types, so far with two different operators, are used by global atmospheric weather model producers.

The global ground-based infrastructure of GNSS receivers reached maturity and a stable number of receivers (e.g. stations of International GNSS Service), with signs of densification of the networks in industrialized regions like Japan, China, Europe, and the USA. The space sector, in particular Spire Global, GeoOptics, Tianmu, PlanetIQ, and Yunyao, are currently outnumbering the public sector organizations, such as EUMETSAT and NOAA, in the quantity of satellites with GNSS sensors.

Inspired by the increasing number of GNSS networks, we have conducted simulations to explore the potential of new observation concepts, based on dense satellite constellation for monitoring the atmospheric state. Therefore, we considered the following configurations: a set of satellites arranged in a strings-of-pearls formation, an extension of the number of satellites in the current orbital planes, and an increase in the number of orbital planes. Simulations were based on Two-Line Element (TLEs) data obtained from Spire Global's Radio Occultation (RO) satellites, and orbit simulations using the FreeFlyer software. We used the in-house developed 3D ray-tracing software in conjunction with the Integrated Tomography (INTOMO) package to reconstruct tropospheric path delays for each RO event and to process them together in an integrated solution using tomographic principles. In this presentation, we analyze the impact of the various satellite configurations on the retrieval of 3D tropospheric refractivity and make use of the simulation results to identify potential new monitoring concepts for future satellite missions.

References:

Acknowledgement of financial support:

Invited Talk - Michael Bussmann

Will data help us to address future challenges?

Michael Bussmann[1]

[1] *Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Center for Advanced Systems Understanding (CASUS), Görlitz, Germany*

m.bussmann@hzdr.de

It has become an often repeated claim that data will be important to address future challenges we are facing. In this talk I will address two distinct cases, health care and energy, and see what the current state of the art of data-driven research is and what obstacles we face to move forward. I argue that data-driven methods have shown siginificant potential to solve problems previously though of being to hard to solve. I will look t two very different cases, personal medicine and fusion, in which very different approaches towards data elucidate why it is important to talk about knowledge rather than data to foster scientific progress. I will end with focusing on what we can improve to move forward in data-driven science.

References:

Acknowledgement of financial support:

Pitch Talk - Artur Yakimovich

Novel Machine Learning Approaches to Study Infection and Disease through Biomedical Images

Artur Yakimovich[1]

[1] *Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Center for Advanced Systems Understanding (CASUS), Görlitz, Germany*

a.yakimovich@hzdr.de

ML and DL are revolutionising our abilities to analyse biomedical images. Among other host-pathogen interactions may be readily deciphered from microscopy data using convolutional neural networks (CNN). We demonstrate in several studies how the definition of novel ML/DL tasks may aid in studying infection and disease phenotypes. Specifically, ML/DL algorithms may allow unambiguous scoring of virus-infected and uninfected cells in the absence of specific labelling. Accompanied by interpretability approaches, the ability of CNN to learn representations, without explicit feature engineering, may allow for uncovering yet unknown phenotypes in microscopy. Furthermore, we demonstrate novel ML/DL approaches to simplified 3D microscopy acquisition using conventional 2D hardware. Finally, we demonstrate how generative AI can be applied to tasks like image reconstruction and resolution enhancement in fluorescence and brightfield microscopy. Taken together, we show novel approaches to established algorithms in Computer Vision and Data Science. Applied to microscopy data, these approaches allow for the extraction of observations from datasets large enough to not be suitable for manual analysis. We argue that this shows that reformulating conventional ML/DL tasks to answer biological questions may facilitate novel discoveries in Infection and Disease Biology.

References:

1. Li, Rui, Mikhail Kudryashev, and Artur Yakimovich. "A weak-labelling and deep learning approach for in-focus object segmentation in 3D widefield microscopy." Scientific Reports 13, no. 1 (2023): 12275.
2. Li, Rui, Gabriel della Maggiora, Vardan Andriasyan, Anthony Petkidis, Artsemi Yushkevich, Mikhail Kudryashev, and Artur Yakimovich. "Microscopy image reconstruction with physics-informed denoising diffusion probabilistic model." arXiv preprint arXiv:2306.02929 (2023).

Acknowledgement of financial support: This work was partially funded by the Center for Advanced Systems Understanding (CASUS) which is financed by Germany's Federal Ministry of Education and Research (BMBF) and by the Saxon Ministry for Science, Culture, and Tourism (SMWK) with tax funds on the basis of the budget approved by the Saxon State Parliament. The authors acknowledge

the financial support by the Federal Ministry of Education and Research of Germany and by Sächsische Staatsministerium für Wissenschaft, Kultur und Tourismus in the programme Center of Excellence for AI-research "Center for Scalable Data Analytics and Artificial Intelligence Dresden/Leipzig", project identification number: ScaDS.AI.

Pitch Talk - Bartosz Brzoza

SE(3)-Transformers for predicting the electronic structure of hydrogen molecules

Bartosz Brzoza[1], Attila Cangi[1]

[1] *Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Center for Advanced Systems Understanding (CASUS), Görlitz, Germany*

b.brzoza@hzdr.de, a.cangi@hzdr.de

In this work, we demonstrate the efficacy of a neural network model implemented as the Materials Learning Algorithms (MALA) package in predicting the electronic structure of a system of hydrogen molecules under various pressure and temperature conditions across the molecular liquid-solid phase boundary, demonstrating the potential of our methods for molecular systems. Additionally, we investigate the use of SE(3)-Transformer Graph Neural Networks to improve the generalizability and extrapolation capabilities of our models. Our results indicate that the MALA framework provides a powerful and efficient tool for accelerating Kohn-Sham density functional theory calculations in molecular systems. This work paves the way for future research in developing advanced machine-learning algorithms for accelerating electronic structure calculations both accurately and efficiently.

References:

Acknowledgement of financial support:

Pitch Talk - Ricardo Martínez García

Dryland conservation as an interdisciplinary problem, or how to combine big data, simulation and mathematical models, and simple experiments to support ecosystem management

Ricardo Martínez García[1]

[1] *Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Center for Advanced Systems Understanding (CASUS), Görlitz, Germany*

r.martinez-garcia@hzdr.de

Water-limited ecosystems are highly complex systems covering 40% of Earth's land surface, mostly in developing countries, and are home to 35% of the world's population. A paradigmatic property of these ecosystems is the spatial self-organization of vegetation, which leads to strikingly regular spatial distributions of plants. These self-organized spatial patterns have been suggested as important ecosystem health indicators. Specifically, pattern shapes may indicate the proximity of the ecosystem to undergo a desertification transition. Despite this potential ecological importance, the plant interactions that underlie pattern formation remain unclear. Without strong empirical evidence of how these patterns emerge, mathematical modeling has been crucial in formulating different hypotheses. However, models assuming different mechanistic origins reproduce the same series of patterns but predict contradicting ecological consequences for them. In this context, a new approach to understanding vegetation dynamics in water-limited ecosystems that focuses on unveiling how plants interact with each other and how those interactions scale to large population sizes to create emergent patterns is needed. In this presentation, I will discuss how to develop such a new approach. I will first present simple mathematical models for pairs of interacting plants that can be parameterized and tested using simple greenhouse experiments. Next, I will discuss how to scale these models to larger system sizes using intensive simulation methods and use them to make predictions about ecosystem-level properties that can be tested with satellite images and remotely sensed vegetation indicators.

References:

1. Cabal, C., Martínez-García, R., de Castro Aguilar, A., Valladares, F., & Pacala, S. W. (2020). "The exploitative segregation of plant roots." Science, 370(6521), 1197-1199.
2. Cabal, C., Maciel, G. A., & Martínez-García, R. (2023). "The evolutionary stability of plant antagonistic facilitation across environmental gradients and its ecological consequences: soil resource engineering as a case study." bioRxiv, 2023-02.
3. Martínez-García, Ricardo, et al. "Integrating theory and experiments to link local mechanisms and ecosystem-level consequences of vegetation patterns in drylands." Chaos, Solitons & Fractals 166

(2023): 112881.

Acknowledgement of financial support:

Sustainability & Circular Economy

Invited Talk - Anna Potysz

Addressing the scientific aspects of a circular economy: insight into secondary resource management

Anna Potysz[1]

[1] *University of Wrocław, Wrocław, Poland*

anna.potysz@uwr.edu.pl

Circular economy constitutes a recently developed strategy which addresses the availability of resources, its consumption and waste generation. According to circular economy assumptions the reduction of wastes and sustainable resource recovery from secondary resources are prioritised. In this regard, scientific contribution to development of sustainable processes dedicated to resource processing is crucial. Metallurgical sector is a key branch supplying metal on a global market. However, apart from economic advantages, this sector also generates wastes such as smelting slags. Such materials however may be efficiently processed provided that appropriate process configuration is defined and designed. Biohydrometallurgical approach is a method which uses microorganisms to extract metals from slags. Such a process is proven efficient provided that metal extraction yield is high and the processing time is as short as possible. This work focused on optimisation of biohydrometallurgical processes applying metallurgical slags of different texture and chemical/phase compo- sition. Various types of bacterial strains were implemented in the leaching process. This strategy aimed to provide a deep insight into behaviour of various slags and to analyse the biotic mechanisms contributing most to metal extraction. Geochemical methods included tracking elements concentration using Inductively cou- pled plasma mass spectrometry and direct surface observations using scanning electron microscopy. Results demonstrated a direct link between solution chemistry and dissolution features occurring on the slag surface which was crucial for understanding what component (phase) is the most susceptible to dissolution under specific biotic conditions. The knowledge acquired from this experimental study allowed to indicate optimal conditions for slag processing. This study highlights that interdisciplinary approaches involving mineralogy, microbiology and geochemistry make a foundation to develop well-designed metal recovery reactors.

References:

Acknowledgement of financial support: This work was financially supported by The National Science Centre (NCN) in Poland in the frame of OPUS25 program under grant agreement 2023/49/B/ST10/01227.

Pitch Talk - Milad Eftekhari

Effect of Ultrafine Particles on Film Stability and Particle Attachment

Milad Eftekhari[1,2], Karin Schwarzenberger[1,2], Kerstin Eckert[1,2]

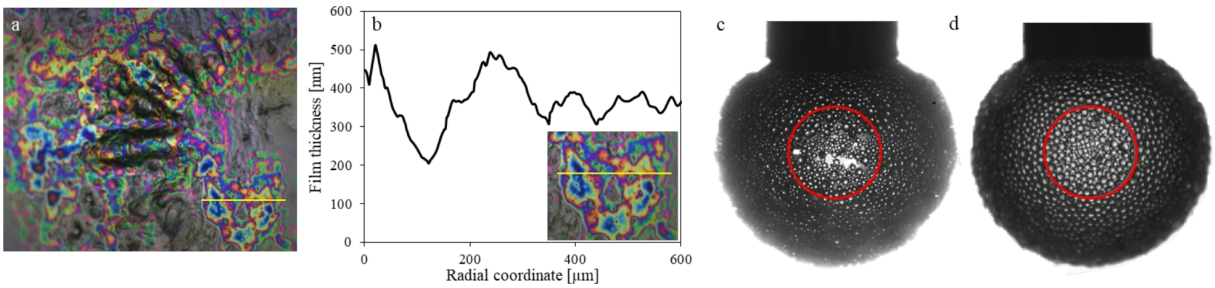
[1] *Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany*

[2] *Technische Universität Dresden, Dresden, Germany*

k.eckert@hzdr.de, k.schwarzenberger@hzdr.de, m.eftekhari@hzdr.de

Froth flotation is an essential separation technique in the mining industry, primarily used to extract valuable minerals from ores. Traditionally, this process targeted particles measuring tens or hundreds of micrometers. However, the recent depletion of high-grade ore deposits has prompted a shift towards exploiting lower-grade mineral deposits. This transition necessitates the fine grinding of ores to effectively liberate the embedded valuable minerals, introducing new challenges associated with managing fine and ultrafine particles.

A notable complication arising from the presence of ultrafine particles is their propensity to excessively stabilize the froth. This excessive stabilization can hinder the flotation process, as overly stable froth impedes the drainage of gangue particles back into the pulp, thus diminishing the grade and selectivity of the concentrate. The stability of the froth is influenced by factors such as the size, hydrophobicity, and shape of the particles. In this study, we investigate the effect of ultrafine particles on the stability of thin liquid films. Through interferometric experiments, we have analyzed how variations in particle concentration and hydrophobicity impact thin film stability. Our findings highlight the significant role of adsorption time on film stability. We categorized the behavior of liquid films with adsorbed ultrafine particles into three distinct types: freshly formed films that ruptured within seconds, films aged for 15 minutes which displayed an extended lifespan with notable thickness variations (Fig. a,b), and films aged for 30 minutes which maintained stability for significantly extended periods 1.



Effect of ultrafine particles on film stability (a interference pattern and b calculated film thickness) and particle distribution on the bubble (c with ultrafine and d without ultrafine).

Furthermore, we investigated the attachment dynamics of coarse particle in the presence of ultrafine particles using a model stirred cell that enables precise control over hydrodynamic conditions 2. Our experiments showed that ultrafine particles not only enhance the attachment rate and probability of coarser particles but also significantly influence the distribution of coarse particles on a bubble surface (Fig. 2 c,d). Additionally, the mobility of coarse particles at the interface changes markedly when ultrafine particles are adsorbed on the bubble surface, which is anticipated to alter the flow structure and flowdriven processes near the bubble, such as the detachment of attached particles.

References:

1. M. Eftekhari, K. Schwarzenberger, S. I. Karakashev, N. A. Grozev, and K. Eckert, "Oppositely charged surfactants and nanoparticles at the air-water interface: Influence of surfactant to nanoparticle ratio," JCIS, 2023, Doi: 10.1016/j.jcis.2023.09.038.
2. M. Eftekhari, K. Schwarzenberger, P. Schlereth, and K. Eckert, "Dynamics of particle attachment in a model stirred cell: A new technique to characterize and quantify particle floatability," Minerals Engineering, 2024, Doi: 10.1016/j.mineng.2024.108643.

Acknowledgement of financial support:

Pitch Talk - Nora Schönberger

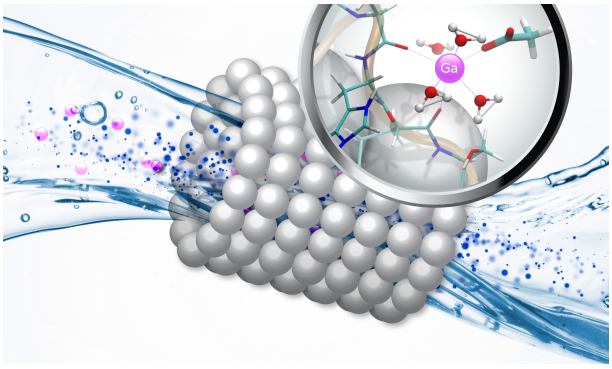
Next-Gen Biosorbents: Peptides for Resource Recovery

Nora Schönberger[1]

[1] *Helmholtz Institute Freiberg for Resource Technology, Freiberg, Germany*

n.schoenberger@hzdr.de

Technological progress and social change are causing an increasing demand for raw materials and a reassessment of traditional methods of resource extraction and waste management. Challenged by environmental impacts and decreasing metal concentrations, traditional mining practices are increasingly seen as unsustainable. This situation is exacerbated by the increasing complexity of primary and secondary raw material sources and decreasing metal content, emphasizing the urgent need for innovative solutions to ensure long-term economic and environmentally sustainable resource provision. Biomining strategies such as biosorption are promising for advancing the circular economy, enabling sustainable resource recovery, and significantly reducing pollution through more effective management of mining and landfill waste.
Among the available biosorption technologies, peptide-based biosorbents are particularly promising. These biosorbents are developed using advanced biotechnological tools such as phage surface display and contain specific peptides that selectively bind the desired metal ions. This precision is critical for the recovery of valuable metals from complex waste streams such as industrial wastewater and e-waste, supporting the principles of the circular economy and improving resource sustainability.



Our research focuses on the development of metal-binding peptides to improve metal recovery processes. Using high-throughput screening and next-generation sequencing, we identify peptides with high specificity and affinity for metals such as cobalt, nickel, arsenic, and others. Using isothermal titration microcalorimetry, these interactions are analyzed in detail, which contributes to understanding binding mechanisms and the optimization of the biosorption process. The newly established junior research group Pep2Rec aims to further develop these biotechnological advances. Pep2Rec aims to refine directed evolution methods to

improve the recovery of metals from non-aqueous solutions. This includes the development of specialized peptide libraries and their application in novel biocomposites for membrane filtration technologies. These initiatives are expected to create a robust framework for a circular economy in sectors with significant potential for improving resource efficiency.

References:

Acknowledgement of financial support:

Pitch Talk - Ashak Mahmud Parvez

Assessment of recyclability of modern printed circuit boards (PCBs) from technical, sustainability and economic perspectives

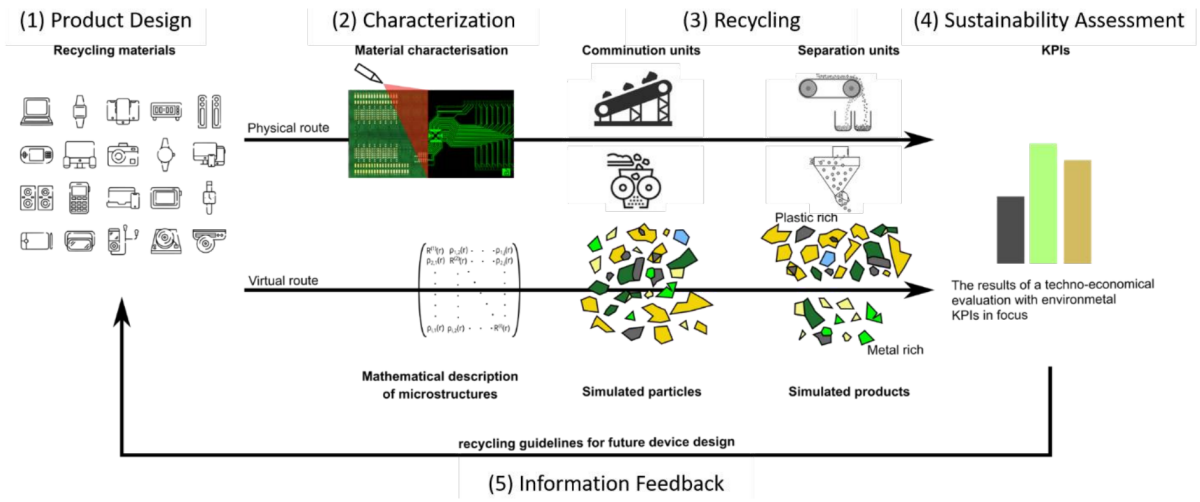
Ashak Mahmud Parvez[1], Peter Boelens[1], Lucas Pereira[1], Robert Moeckel[1], K. Gerald van den Boogaart[1], Lucas Ott[2], Frank Ellinger[2], Yana Vaynzof[2], Christina Dornack[2], Jens Gutzmer[1]

[1] *Helmholtz-Zentrum Dresden - Rossendorf (HZDR), Dresden, Germany*

[2] *Technische Universität Dresden, Dresden, Germany*

p.boelens@hzdr.de, a.parvez@hzdr.de, l.pereira@hzdr.de, lucas.ott@tu-dresden.de, r.moeckel@hzdr.de, yana.vaynzof-@tu-dresden.de, christina.dornack@tu-dresden.de, frank.ellinger@tu-dresden.de, j.gutzmer@hzdr.de, boogaart-@hzdr.de

The development of concepts for the comprehensive recycling of end-of-life printed circuit boards (PCBs) is challenging because of their complex composition and the minute scale of the electronic components used. This is due to the fact that PCB design mostly considers achieving pre-defined performance indicators at lowest possible cost. Recyclability considerations, on the other hand, are still of little relevance to PCB design. This is despite the fact that recyclability will be imperative to reach the sustainability goals set by society. Achieving these goals may, in turn, demand important changes in PCB design strategies.



Schematic diagram of overall study: (1) product design, (2) characterization, (3) recycling, (4) sustainability assessment and (5) information feedback.

Based on the above, the recyclability of state-of-the-art PCBs is critically assessed in a current investigation. This investigation takes into account a wide range of circular economy aspects (e.g. minimization of

resource consumption, reduction of toxic materials in production, and enhancement of recycling rate). The study places a particular focus on the opportunity to mechanically separate metals and plastics fractions using a comprehensive suite of mechanical separation technologies. These technologies exploit different physical properties of metals and plastics, e.g., density, magnetic susceptibility or conductivity. The separation efficiency and limitations of each of these technologies is assessed with particle-based separation models, accounting for the size, shape, and composition of particles in the experiments. The recyclability potential is then evaluated from exergy and life-cycle assessment perspectives. HSC Sim and openLCA software packages are used in combination for this task. Overall, the finding of this study will provide PCB designers with important insight on possible recycling rates, material selection, energy consumption during recycling and the environmental footprint of modern PCBs.

References:

Acknowledgement of financial support:

Pitch Talk - Mateusz Kruszelnicki

Sustainable flotation solutions: Investigating the impact of biological origin surfactants on bubble-particle interactions

Mateusz Kruszelnicki[1], Krzysztof Legawiec[1], Pavlina Basarova[2], Jan Zawala[3], Michalina Zawadzka[4], Izabela Polowczyk[1]

[1] *Wrocław University of Science and Technology, Wrocław, Poland*

[2] *University of Chemistry and Technology, Prague, Czech Republic*

[3] *Jerzy Haber Institute of Catalysis and Surface Chemistry Polish Academy of Sciences, Kraków, Poland*

[4] *University of Wroclaw, Wrocław, Poland*

krzysztof.legawiec@pwr.edu.pl, mateusz.kruszelnicki@pwr.edu.pl

Froth flotation is a selective separation process based on the differences in surface properties of the mineral particles. The desired modification of surface properties is achieved through the addition of surface-active substances. The vast majority of currently employed chemicals are of synthetic origin. Therefore, efforts are being made to replace them with natural, biodegradable equivalents, such as those produced by microorganisms. Biosurfactants are more beneficial than synthetic surfactants in terms of high biodegradability, lower toxicity, environmental compatibility and production from renewable sources – advantages that synthetic surfactants do not exhibit.

Our research aimed to determine how Rhamnolipid biosurfactant (RL) produced by Pseudomonas aeruginosa affects the fundamental act of the flotation, i.e. bubble-particle attachment. The process of air bubble adhesion to the surface of a solid with varying degrees of hydrophobicity was evaluated at different concentrations of RL, up to 500 mg dm^{-3}, both at pH 5 (RL non-ionic form) and pH 10 (RL anionic form).

The dependence of the three-phase contact (TPC) formation time on biosurfactant concentration was determined by monitoring the bubble-solid surface interactions using a high-speed camera. It was found that as the concentration of RL rises, the time needed for TPC formation extends as a result of an increase in the film drainage time. A significant effect of RL on the TPC line expansion (lower rate) and the size of the contact area between the bubble and the surface (smaller surface area) was also noted. At excessively high concentrations, the use of rhamnolipid biosurfactant in flotation could potentially hinder flotation kinetics and efficiency due to its strong foaming action. These effects will be of particular importance for the actual flotation process, in which this biosurfactant would be used as a collector or frothing agent.

References:

Acknowledgement of financial support: This study was financed by National Science Centre (Poland)

Research Grant No. 2019/33/N/ST8/03026 and CEEPUS-NAWA programme (CIII-Freemover-2122-152212

Pitch Talk - Krzysztof Legawiec

Development of functionalized cellulose nanostructures for controlled and efficient aggregation of fine mineral particles towards sustainable mineral engineering

Krzysztof Jan Legawiec[1], Mateusz Kruszelnicki[1], Radosław Stanisławski[1], Dominika Benkowska-Biernacka[1], Agnieszka Gawin-Mikołajewicz[2], Izabela Polowczyk[1]

[1] *Wrocław University of Science and Technology, Wrocław, Poland*

[2] *Wrocław Medical University, Wrocław, Poland*

dominika.benkowska@pwr.edu.pl, mateusz.kruszelnicki@pwr.edu.pl, agnieszka.gawin-mikolajewicz@umw.edu.pl, radoslaw.stanislawski@pwr.edu.pl, izabela.polowczyk@pwr.edu.pl, krzysztof.legawiec@pwr.edu.pl

Cellulose-based chemicals attract significant attention from researchers not only in fundamental research but also as potential replacements for petroleum-based chemicals in industrial applications. The primary challenge to scaling up the use of functionalized cellulose nanomaterials lies in developing economically viable fabrication methods.

In the two-step reaction that produces amine-functionalized cellulose, with an intermediate step to obtain 2,3-dialdehyde cellulose, critical parameters include the quantities of oxidizing and reducing agents. By optimizing these synthesis parameters, it is possible to reduce the demand for media and chemicals, particularly oxidation reagents (sodium periodate) and the reducing agent (2-picoline-borane). Additional variables include residence time in the reactor and the temperature. Naturally, the correlation of all these parameters directly impacts the efficiency of the process.

In our study, we modelled these correlations using statistical experimental design (DOE) and radial basis neural network (RBNN) techniques. The resulting models facilitated the production of cellulose structures with varying degrees of substitution by amine functional groups (n-alkylamines, C2-C8), aiming to maximize reaction yield while minimizing the consumption of oxidation and reduction agents. The functionalized fibres were subsequently homogenized to nanometric size using high-pressure homogenization.

Finally, the stability of suspensions of fine mineral particles (galena, pyrite, chalcocite, and quartz) in the presence of these nanostructures was assessed using the multiple light scattering (MLS) technique. The morphology of the resulting aggregates was analysed using optical microscopy with numerical image analysis.

Our results demonstrate basic characteristics of the flocculation process, laying the groundwork for further research aimed at optimizing and controlling the selectivity of the process in polymineral suspensions.

References:

Novel Materials

Invited Talk - Rico Friedrich

Data-driven Design of Novel Ionic Two-dimensional and High-entropy Materials

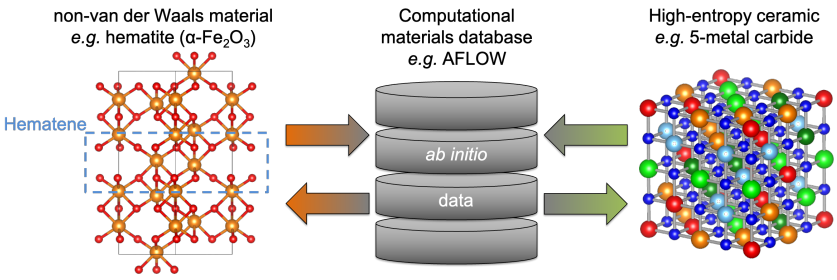
Rico Friedrich[1]

[1] *Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany*

r.friedrich@hzdr.de

The design of novel materials for various scientific and technological applications has in recent years benefitted from the introduction of data-driven methods. Here, this will be demonstrated for two exemplary materials classes.

While two-dimensional (2D) materials are traditionally derived from bulk layered compounds bonded by weak van der Waals (vdW) forces, the recent surprising experimental realization of non-vdW 2D compounds obtained from non-layered crystals [1] foreshadows a new direction in 2D systems research. We present several dozens of candidates of this novel materials class derived from applying data-driven research methodologies in conjunction with autonomous ab initio calculations [2,3]. Surface passivation of these systems can be used to control their magnetic state and eventually even to induce ferromagnetism [4]. The candidates thus exhibit a wide range of appealing electronic, optical and magnetic properties making them an attractive platform for fundamental and applied nanoscience.



Also high entropy materials have recently attracted significant interest due to their favorable mechanical, catalytic, and electronic properties. High-entropy ceramics consist of an ordered anion sublattice of carbon, nitrogen or oxygen and a disordered cation sublattice maximizing configurational entropy by randomly occupying it by five or more cation species (transition metal elements). The reliable computational modelling of such systems can be realized by expanding it into a large ensemble of ordered structures [5]. For the actual manufacturing of high-entropy materials, predictive synthesizability descriptors such as the entropy-forming ability (EFA) [6] and the disordered enthalpy-entropy descriptor (DEED) [7] are crucial prerequisites. We present here extensive results validating the predictive power of these approaches. These findings thus pave the way towards an efficient computational design of high-entropy compounds for extreme conditions.

References:

1. A. Puthirath Balan et al., Nat. Nanotechnol. 13, 602 (2018).
2. R. Friedrich et al., Nano Lett. 22, 989 (2022).
3. T. Barnowsky et al., Adv. Electron. Mater. 9, 2201112 (2023).
4. T. Barnowsky et al., Nano Lett. 24, 3874 (2024).
5. K. Yang et al., Chem. Mater. 28, 6484 (2016).
6. P. Sarker et al., Nat. Commun. 9, 4980 (2018).
7. S. Divilov et al., Nature 625, 66 (2024).

Acknowledgement of financial support: Funding from the German Research Foundation (DFG), project FR 4545/2-1, and for the "Autonomous Materials Thermodynamics" (AutoMaT) project by Technische Universität Dresden and Helmholtz-Zentrum Dresden-Rossendorf within the DRESDEN-concept alliance is gratefully acknowledged.

Pitch Talk - Agnieszka Kuc

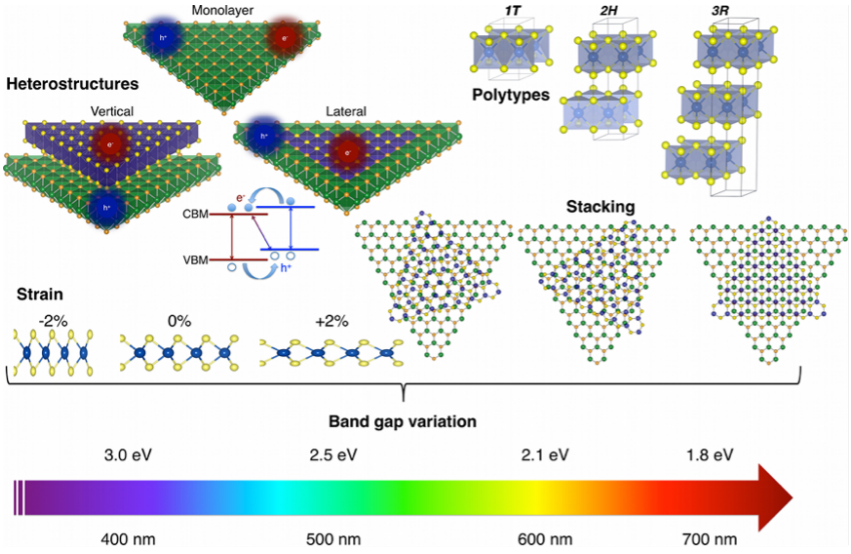
Two-dimensional materials for applications in chemistry, physics, and materials science

Agnieszka Kuc[1]

[1] *Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Center for Advanced Systems Understanding (CASUS), Görlitz, Germany*

a.kuc@hzdr.de

Van der Waals (vdW) 2D materials are found in various polytypes and can easily be exfoliated into monolayers. Stacking different single layers on top of each other creates heterostructures, which exhibit intriguing chemical and physical properties. These properties include the formation of moiré structures or interlayer excitons, among others. The characteristics of such vdW systems can further be fine-tuned through external factors, such as applied electric fields, tensile strain, or the twist angle between layers. Within our research group, we focus on the exploration of 2D vdW materials, including transition-metal dichalcogenides, graphene, and 2D polymers, just to mention a few. We investigate their potential applications in fields, such as (opto)electronics, hydrogen isotope sieving and transport, and catalysis. These materials hold particular significance for these applications because they confine electrons to two dimensions. Additionally, their properties are distinct from those of their bulk parent systems and are uniquely manifested at such lower dimensions. I will present some of the most recent investigations carried out in the group, which are also part of two ongoing projects, Collaborative Research Center CRC1415 and Research Training Group RTG 2721.



References:

Acknowledgement of financial support: Financial support by DFG within Collaborative Research Center CRC1415 and Research Training Group RTG 2721.

Pitch Talk - Joanna Grzyb

Nanomaterials - a platform or a cargo in a delivery into a living cell

Szymon Nowak[1], Patryk Majka[1], Jakub Sławski[1], Joanna Grzyb[1]

[1] *University of Wroclaw, Wrocław, Poland*

joanna.grzyb@uwr.edu.pl

Nanomaterials are a broad class of materials, defined simply by their size reduced to nanometers in at least one of their dimensions. The type of nanomaterials are nanoparticles, reduced in all their dimensions to not more than 100 nm. Most of the nanoparticles are not bigger than 10 nm. Such size reduction results in the gaining of new electronic properties, being an effect of quantum confinement. The best known is the ability of fluorescence obtained by semiconductor material after becoming quantum dots (QD). QDs are used as fluorescent labels, and also as partners in energy and electron transfer. Some of the carbon-based nanomaterials are also fluorescent. On the other side, there are carbon nanotubes, relatively huge nanostructures, that can be used as a platform for obtaining a junction of other elements on their surface. In general, joining nanomaterials and biological elements may lead to obtaining a new functionality - a nanobiohybrid. In our research group, we tend to obtain the nanohybrids, that can be further used for light-controlled triggering of a desired metabolic process. For that, we need e.g. a redox active element to be delivered into a proper cell compartment. Such redox-active elements might be e.g. QD, or redox-active proteins, linked to a carbon nanotube surface. Here, we present our strategy of targeting QD to mitochondria by attaching protein with mitochondria-specific target peptide, and test of efficiency of this nanohybrid delivery into a living cell and isolated mitochondria. We also present the protein-QD junction on the surface of carbon nanotubes, as well as the test of their delivery to the living cells. Although we are far from light-controlling of life, we might be a step forward.

References:

Acknowledgement of financial support:

Pitch Talk - Justyna Zeler

Exploring Thermoluminescence and Luminescence Thermometry Processes in Phosphors

Justyna Zeler[1], Dominika Grzesiak[1], Aleksandra Małoń[1], Aleksandra Owczarek[1], Eugeniusz Zych[1], Luis D. Carlos[2]

[1] *University of Wroclaw, Wrocław, Poland*

[2] *University of Aveiro, Aveiro, Portugal*

eugeniusz.zych@uwr.edu.pl, justyna.zeler@uwr.edu.pl

Multifunctional phosphors play an important role across diverse fields, from lighting to biomedical applications. Through the utilization of thermoluminescence and luminescence thermometry techniques, we aim to unravel and regulate the intricate luminescent behaviors of these phosphors.

Our research delves into exploring the thermometric and thermoluminescent characteristics of Cr^{3+}-activated aluminate materials, particularly focusing on the impacts of co-doping with various lanthanide ions. Through meticulous analysis, we seek to elucidate how lanthanide co-doping influences the temperature response and thermoluminescent properties of these phosphors, providing valuable insights for their utilization in nanomedicine applications.

References:

Acknowledgement of financial support: The research finances by the Polish National Science Centre under OPUS grant #UMO2023/49/B/ST5/04265.

Pitch Talk - Eugeniusz Zych

When Luminescence Thermometry Can Compete with Pyrometry?

Eugeniusz Zych[1], Justyna Zeler[1], Dagmara Kulesza[1], Paulina Bolek[1], Joanna Trojan-Piegza[1], Pola Łukaszczuk[1], Małgorzata Sójka[2]

[1] *University of Wroclaw, Wrocław, Poland*

[2] *General Electric & University of Wroclaw, Wrocław, Poland*

eugeniusz.zych@uwr.edu.pl, paulina.bolek@uwr.edu.pl, dagmara.kulesza@uwr.edu.pl, 338803@uwr.edu.pl, joanna.trojan-piegza@uwr.edu.pl, justyna.zeler@uwr.edu.pl, malgorzata.sojka@ge.com

Luminescence thermometry is sometimes viewed and presented in contrast to pyrometry. This does not seem appropriate, as both techniques have significant advantages but also limitations. When considering whether luminescence thermometry can compete with pyrometry, it is essential to evaluate the application's specific requirements, such as temperature range, measurement environment, and desired accuracy and sensitivity.

Luminescence thermometry, a noninvasive remote technique, is remarkably adaptable, making it suitable for measuring temperatures in environments where direct contact is not feasible or safe. Depending on the luminescent material used, it can cover a broad temperature range, from cryogenic to high temperatures. This adaptability, however, can be a challenge. A single material rarely can offer temperature measurement over a truly broad range. Yet, this method can present high spatial resolution, enabling temperature mapping of surfaces with fine detail.

However, choosing luminescent material is critical, and not all materials are suitable for all temperature ranges or environments. It's important to note that luminescence thermometers require careful calibration against known temperatures or standards. This process can be time-consuming and labor-intensive and may need to be done repeatedly. Environmental conditions such as ambient light, humidity, and contaminants can affect luminescence properties, potentially impacting the accuracy of measurements.

In this presentation, we shall show that luminescence thermometers can offer good-quality measurements over a wide range of temperatures, from helium up to about 1000 °C. Therefore, this technique might be a better choice in such circumstances than pyrometers. The choice of the activator and the host to design a luminescence thermometer presenting good sensitivity in the required range of temperatures will be discussed.

References:

Acknowledgement of financial support: The Polish National Science Centre (NCN) financed the research under OPUS grant #2018/31/B/ST4/00924.

Pitch Talk - Hossein Tahmasbi

An Automated Materials Discovery Approach with Machine Learning

Hossein Tahmasbi[1], Attila Cangi [1], Kushal Ramakrishna[2], Mani Lokamani[2]

[1] *Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Center for Advanced Systems Understanding (CASUS), Görlitz, Germany*

[2] *Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany*

a.cangi@hzdr.de, m.lokamani@hzdr.de, k.ramakrishna@hzdr.de, h.tahmasbi@hzdr.de

A comprehensive potential energy surface (PES) exploration is an essential ingredient for the discovery of novel phases with potential technological importance. This can be achieved using transferable machine-learned interatomic potentials (ML-IAPs), which are trained and validated using automated workflows enabling efficient simulations of large systems.

Here, we demonstrate this methodology by investigating iron hydride (FeH) phases across a pressure range of 0-100 GPa. We utilize the PyFLAME code [1] for ML-IAP construction and perform a comprehensive global sampling of FeH structures using the minima hopping method [2]. Apart from identifying the experimentally established *dhcp*, *hcp*, and *fcc* phases of FeH, we uncover a multitude of novel low-enthalpy structures, including modified and stacking fault variants of known FeH phases [3]. These findings highlight the ability of ML-IAPs coupled with large-scale structure prediction to reveal a rich landscape of stable and metastable materials.

References:

1. H. Mirhosseini, H. Tahmasbi, S. R. Kuchana, S. A. Ghasemi, and T. D. Kühne, Comput. Mater. Sci. 197, 110567 (2021).
2. M. Amsler and S. Goedecker, J. Chem. Phys. 133, 224104 (2010).
3. H. Tahmasbi, K. Ramakrishna, M. Lokamani, and A. Cangi, Phys. Rev. Mater. 8, 033803 (2024).

Acknowledgement of financial support:

Digital Health & Life Sciences

Invited Talk - Elżbieta Gumienna-Kontecka

Harnessing the power of microbial siderophores for nuclear imaging

Elżbieta Gumienna-Kontecka[1]

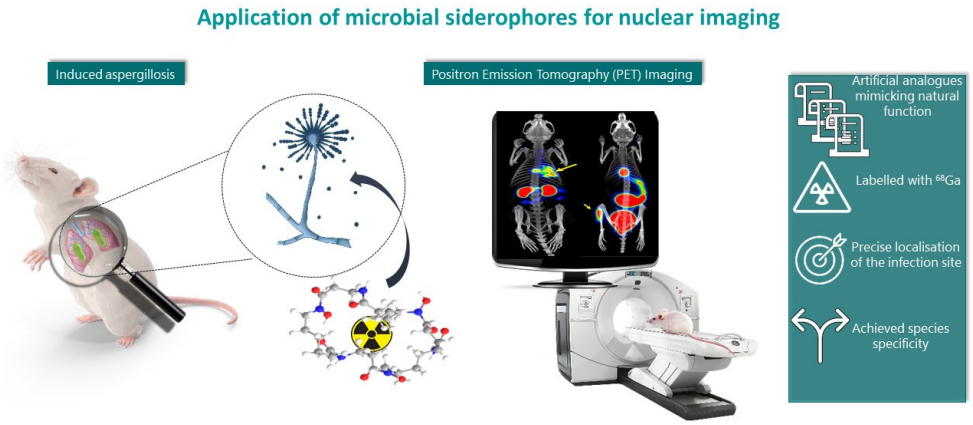
[1] *University of Wroclaw, Wrocław, Poland*

elzbieta.gumienna-kontecka@uwr.edu.pl

Under iron-deficient conditions most aerobic microorganisms secret low molecular-weight chelating compounds – siderophores, which actively transport ferric ions into the cells via specific transporters in the microbial membranes [1, 2]. The biomimetic approach allowed us to diversify the arsenal of siderophore-type molecules, introduce additional desired chemical and/or physical properties, and provide means to identify general motifs governing an interplay between structure and function in biological activity [1-5].

Taking into account, that siderophores are absent in the host cells, they are tempting targets for microbial imaging, for example with Ga-68 or Zr-89 using positron emission tomography (PET) [6]. Of the evaluated siderophores, 68Ga-ferrioxamine E and its close biomimetic analogues were shown as the most promising for possible applications in PET imaging of S. aureus and A. fumigatus species [7]. Currently we are working on other bacterial (P. aeruginosa) and fungal species, to better understand the in vivo speciation and differences in the biological recognition and uptake.

On the other hand, desferrioxamine B (DFO) is currently the most commonly used chelator to radiolabel biomolecules with 89Zr [6]. However, its in vivo stability has proven insufficient, and transchelation has been observed. Our Zr(IV) – DFO solution studies provided information on the actual chemical form of the complex in biological media [8], and this can contribute to a better understanding of the in vivo speciation and differences in the biological activity of this and other chelators [5-7].



Overall, mimics of siderophores hold potential as inert and stable carriers for Fe(III), Ga(III) and Zr(IV) ions for diagnostic medical applications. They also allow identifying critical microbial compartments in which siderophores accumulate and thus illuminate key targets for specific drugs against microbial diseases.

References:

1. A. Szebesczyk, E. Olshvang, A. Shanzer, P.L. Carver, E. Gumienna-Kontecka, Coord. Chem. Rev., 2016, 84, 327.
2. A. Mular, K. Piasta, A. Jedyńczuk, K. Kamińska, E. Olshvang, N. Metzler-Nolte, E. Wojaczyńska, H. Kozłowski, E. Gumienna-Kontecka, Coord. Chem. Rev., 2024, 501, 215551/1.
3. E. Olshvang, A. Szebesczyk, H. Kozłowski, Y. Hadar, E. Gumienna-Kontecka, A. Shanzer, Dalton Trans. 2015, 44, 20850.
4. J. Besserglick, E. Olshvang, A. Szebesczyk, J. Englander, D. Levinson, Y. Hadar, E. Gumienna-Kontecka, A. Shanzer, Chem. Eur. J. 2017, 23, 13181.
5. Y. Toporivska, A. Mular, K. Piasta, M. Ostrowska, D. Illuminati, A. Baldi, V. Albanese, S. Pacifico, I.O. Fritsky, M. Remelli, R. Guerrini, E. Gumienna-Kontecka, Inorg. Chem. 2021, 60, 13332.
6. M. Petrik, Ch. Zhai, H. Haas, C. Decristoforo, Clin. Transl. Imaging, 2017, 5, 15.
7. A. Mular, A. Shanzer, H. Kozłowski, I. Hubmann, M. Misslinger, J. Krzywik, C. Decristoforo, E. Gumienna-Kontecka, Inorg. Chem. 2021, 60, 17846.
8. Y. Toporivska, E. Gumienna-Kontecka, J. Iorg. Biochem., 198 (2019) 110753/1.

Acknowledgement of financial support: The research has received funding from Polish National Science Centre (UMO-2017/26/A/ST5/00363 and UMO-2022/47/I/ST4/02354).

Pitch Talk - Ellen Adams

Cation Specific Stabilization of FUS Biomolecular Condensates

Ellen Adams[1]

[1] *Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany*

e.adams@hzdr.de

Biomolecular condensates have been linked to the neurodegenerative diseases, where the transition from a liquid-like to solid-like phase results in formation of irreversible protein aggregates. Yet, the molecular organization within condensates remains largely unknown. Here, the link between environmental conditions and phase separation of intrinsically disordered proteins are explored. The influence of salt concentration on the organization of condensates made from FUS protein is investigated, with a focus on biologically relevant chloride salts with Na^+, K^+, Mg^{2+}, and Ca^{2+} counter ions. Attenuated total reflection THz (ATR-THz) spectroscopy is utilized to probe the intermolecular vibrational modes of the water hydrogen-bonding network, which reveals the structure and dynamics of protein hydration within condensates. In this study, results indicate that the hydration of FUS proteins is significantly perturbed by salt concentration, but is not cation specific. The strength of the hydrogen bonding network, however, is cation specific, and a weaker water network is observed for monovalent cations relative to divalent cations. Here, we reveal that the stability of biomolecular condensates is impacted by the presence of specific ions, ultimately shedding light on the molecular properties that dictate the organization of condensates.

References:

Acknowledgement of financial support:

Pitch Talk - David Pape

METABOLATOR: Establishing a Citable Web Application for Automated Metabolic Load Analysis

David Pape[1], Mani Lokamani[1], Ayush Seal[1], Oliver Knodel[1], Jeffrey Kelling[1], Karim Fahmy[1], Guido Juckeland[1]

[1] *Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany*

d.pape@hzdr.de, j.kelling@hzdr.de, o.knodel@hzdr.de, m.lokamani@hzdr.de, g.juckeland@hzdr.de

METABOLATOR is a web application for automated analysis of microcalorimetric metabolic data using Monod's equation. The software was developed in collaboration between the Institute of Resource Ecology and the Department of Information Services and Computing at Helmholtz-Zentrum Dresden - Rossendorf (HZDR), and is now offered as a web service for the community. In addition to publishing the software under an open source license, we made the service, which is hosted on HZDR infrastructure, citable by registering its metadata with DataCite and minting a dedicated Digital Object Identifier (DOI). In this talk, we will present the results of our collaboration from the point of view of a Research Software Engineer (RSE). We will introduce the METABOLATOR software, and discuss its development from initial trials into an installable package and web service. Moreover, we will debate the importance of persistent identifiers (PIDs) for reproducible, citable, and overall FAIR data analysis workflows.

References:

Acknowledgement of financial support:

Pitch Talk - Xinne Zhao

Droplet-Based Microfluidics for Point-of-Care Monitoring of Biomarker Levels in Clinical Diagnostics

Xinne Zhao[1], Fiona R. Kolbinger[2], Lars Heubner[2], Larysa Baraban[1], Tom A. Schröder[2]

[1] *Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany*

[2] *Technische Universität Dresden, Dresden, Germany*

l.baraban@hzdr.de, fiona.kolbinger@uniklinikum-dresden.de, tom.schroeder@ukdd.de, lars.heubner@ukdd.de, x.zhao-@hzdr.de

Biomarkers play an important role in early detection and prognosis; evaluating and monitoring their levels can indicate various clinical conditions of diseases (e.g., cancer and metabolic disorders).1 However, the traditional diagnostic methods often involve time-consuming laboratory assays, delaying clinical decisions. In recent years, there has been a growing interest in developing portable point-of-care diagnostic tools for rapid and accurate detecting of biomarkers.2 However, these biomolecular tests mainly focus on detecting biomolecules intermittently, lacking real-time and continuous monitoring. In our group, we present a novel portable droplet-based microfluidic system, combined with optical sensors, for the real-time continuous and long-term monitoring of biomarker (amylase or lactate) levels. Based on encapsulating samples within discrete droplets, our platform integrates sample acquisition, enzymatic assays, and optical detection, enabling real-time monitoring of biomarker concentrations with minimal sample volumes, reagent dose, and processing time. Moreover, our approach can analyze diverse clinical samples, including blood, interstitial fluids, and drain liquid with high sensitivity, selectivity, and accuracy. In previous work, we have achieved real-time sensing of drain α-amylase activity of patients undergoing pancreatic surgery with a bedside portable droplet-based millifluidic device.3 Among 32 patient samples, 97% of the results matched the clinical data. This strategy significantly improves the determination time (3 min), the detection limit of 7 nmol/s $\cdot$ L, and minimal material requirement (ca. 10 μL) and wastes. In the latest work, the portable droplet-based strategy performed well in accurately tracking lactate levels in the blood and interstitial liquid during animal trials, which aims to locally monitor lactate levels to indicate tissue blood perfusions during skin graft surgery. In summary, the droplet-based platform used in biomarkers monitoring brings a big potential in medical diagnosis, disease monitoring, peri-, and postoperative monitoring, and metabolism tracking during exercise.

References:

1. Qiu, Shi, et al. "Small molecule metabolites: discovery of biomarkers and therapeutic targets." Signal Transduction and Targeted Therapy 8.1 (2023): 132.

2. Natalia, Auginia, et al. "Analytical device miniaturization for the detection of circulating biomarkers." Nature Reviews Bioengineering 1.7 (2023): 481-498.
3. Zhao, Xinne, et al. "Portable droplet-based real-time monitoring of pancreatic α-amylase in postoperative patients." Biosensors and Bioelectronics 251 (2024): 116034.

Acknowledgement of financial support: The financial support of the project ImmunoChip which has received funding from the European Research Council (ERC) under the European Union's Horizon Europe research and innovation programme grant agreement No 101045415.

Pitch Talk - Željko Janićijević

Multiplexed Extended-Gate Field-Effect Transistor Biosensing Systems: Powerful and Cost-Effective Tools for the Future of Digital Healthcare

Željko Janićijević[1], Trang-Anh Nguyen-Le[1], Isli Cela[1], Michael Bachmann[1], Larysa Baraban[1]

[1] *Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany*

l.baraban@hzdr.de, z.janicijevic@hzdr.de

Electronic biosensors have found numerous applications in point-of-care (POC) diagnostics thanks to their affordability and facile integration into portable devices, enabling rapid digital display of measured data. However, this class of biosensors still did not reach the stability and reliability required for demanding healthcare applications, such as the diagnostics of complex diseases or therapy monitoring, where multiple biomarkers need to be measured simultaneously with high accuracy and sensitivity. In these application scenarios, multiplexing represents a promising practical solution enabling simultaneous and reproducible measurements at many sensing points, as well as robust statistics. Extended gate (EG) field-effect transistor (FET) biosensor systems are excellent candidates for multiplexed sensing of various physiologically relevant (bio)chemical analytes, from ions to biomolecules. The FET transducer endows the system with exceptional sensitivity and straightforward interfacing with readout electronics, while the physical separation of the gate electrode from the transducer facilitates the integration of multiple individually tailored sensing points into the compact, disposable, and cost-effective sensing interface with versatile architectures [1]. We have demonstrated multiplexed, portable, and standalone EG-FET biosensing platforms combining the optimized design of conventional electronics based on off-the-shelf components and different innovative assay strategies, thereby achieving remarkable detection limits for biomolecules, improved by several orders of magnitude compared to clinical gold standard ELISA assays. Using gold nanoparticle analyte labels as nanoantennae, we realized a highly sensitive POC immunosensor [2]. Moving beyond the traditional POC diagnostics applications, we implemented an indirect assay methodology enabling the detection of target molecules relevant for monitoring cancer immunotherapy [3]. Our EG-FET platforms offer a great opportunity for advanced digitalized healthcare screening and monitoring by quickly providing more comprehensive information to clinicians. They can be easily upgraded to support data connectivity and effective incorporation of artificial intelligence. We envision EG-FET biosensing platforms as important components of future digital health ecosystems.

References:

1. Ž. Janićijević, T.-A. Nguyen-Le, and L. Baraban, "Extended-gate field-effect transistor chemo- and biosensors: State of the art and perspectives", Next Nanotechnology, vol. 3–4, p. 100025, Sep. 2023,

doi: 10.1016/j.nxnano.2023.100025.

2. Ž. Janićijević, T.-A. Nguyen-Le et al., "Multiplexed extended gate field-effect transistor biosensor with gold nanoantennae as signal amplifiers", Biosensors and Bioelectronics, vol. 241, p. 115701, Dec. 2023, doi: 10.1016/j.bios.2023.115701.
3. T.-A. Nguyen-Le et al. "Towards precision immunotherapy: FET biosensors for immunotherapeutic drug monitoring in UniCAR T-cell therapy", Manuscript in preparation.

Acknowledgement of financial support: This research was supported by the European Research Council (ERC) Consolidator Grant (ImmunoChip, ID: 101045415).

Pitch Talk - Olga Michel

Anti-SARS-CoV-2 platform based on maleimide-functionalized liposomes

Olga Michel[1], Aleksandra Kaczorowska[1], Lucyna Matusewicz[1], Kliwia Piórkowska[2], Marlena Golec[2], Adam Konka[2], Joanna Zembala-John[3,4], Aleksander F. Sikorski[4], Aleksander Czogalla[1]

[1] *University of Wroclaw, Wrocław, Poland*

[2] *Silesian Park of Medical Technology Kardio-Med Silesia, Zabrze, Poland*

[3] *Medical University of Silesia, Zabrze, Poland*

[4] *Acellmed Ltd., Zabrze, Poland*

a.konka@kmptm.pl, m.golec@kmptm.pl, olga.michel@uwr.edu.pl, aleksander.sikorski@uwr.edu.pl, aleksandra.kaczorowska@uwr.edu.pl, aleksander.czogalla@uwr.edu.pl, jzembala@wp.pl, lucyna.matusewicz2@uwr.edu.pl, k.piorkowska@kmptm.pl

The rapid spread of the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) has led to an unprecedented public health crisis worldwide. The intensive work on vaccine development, prompted by the COVID-19 pandemic, has led to milestone achievements in mRNA and liposome-based technologies and raised the general interest in lipid nanocarriers. However, due to the limitation of vaccine-induced immunity as well as the emergence of new virus mutations, the challenge remains to develop specific, targeted drugs that inhibit the progression of the infection. In response to that call, we developed a platform against the SARS-CoV-2 virus using maleimide-functionalized liposomes, inhibiting the viral binding with the ACE2 receptor, thus blocking the infection progression. A polyethylene glycol molecule containing a maleimide functional group was used to immobilize a short peptide sequence with high affinity towards the viral spike protein. To ensure high homogeneity and long-term stability of peptide-liposome preparations, extensive optimizations were made towards e.g. lipid composition of the nanocarrier and manufacturing approaches. We found that changes in cholesterol content and using various phosphatidylglycerol species not only affect long-term stability but also alter the functionality of peptide-liposome formulations in vitro. We used two techniques to calibrate liposomes: a high-pressure homogenization and extrusion. Although better parameters were achieved with the latter, after optimization of liposome composition both techniques allowed to generate homogeneous, stable preparations. The inhibitory effect of the peptide-liposomal preparation was confirmed in vitro on ACE2-expressing cells using a syncytia-forming assay and a luciferase-labeled pseudovirus. In addition to the anti-SARS-CoV-2 peptide, the same maleimide-functionalized liposomes were used to immobilize the anti-influenza peptide. Based on elaborated techniques and protocols, equally stable formulations were obtained, demonstrating our maleimide-based liposomal platform's great potential against COVID-19, influenza, and other infections caused by RNA viruses.

References:

Acknowledgement of financial support: Funding sources: Project number 2021/ABM/05/00002-00 financed by the Medical Research Agency, Poland. Project title: "Mutation-resistant nano therapeutics inhibiting infection progress of RNA-virus, SARS-CoV-2"

Posters

$NiPS_3$ and $CrPS_4$ – The interplay between structure and magnetic ordering

Beatriz Costa Guedes[1], Agnieszka Kuc[1], Andrea Leon[2], Thomas Brumme[3], Thomas Heine[1,3]

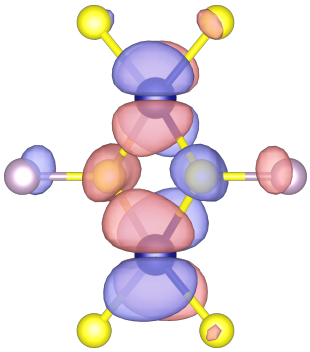
[1] *Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Center for Advanced Systems Understanding (CASUS), Görlitz, Germany*

[2] *University of Chile, Chile*

[3] *Technische Universität Dresden, Dresden, Germany*

b.costa-guedes@hzdr.de, a.kuc@hzdr.de, thomas.heine@tu-dresden.de, thomas.brumme@mailbox.tu-dresden.de, andrea.leon@uchile.cl

Magnetic van der Waals materials, such as transition metal phosphorous chalcogenides MPS_3 and MPS_4 (M = Mn, Fe, Co, and Ni), offer potential for coupled spintronic and optoelectronic applications due to their wide band gap (1.2 - 3.5 eV) [1] and efficient light absorption. While both belong to the C2/m space group, they differ in magnetic ordering, with MPS_3 preserving antiferromagnetic (AFM) ordering [1] and $CrPS_4$ changing from AFM to ferromagnetic (FM) in the monolayer limit [2]. However, the mechanism and role of exchange interaction still need to be clarified, especially in the case of MPS_4. Our methodology involved using VASP with PAW and PBE+D3, optB86-vdW functionals, and the SCAN functional. For the magnetic structure, we adopted the GGA+U approach with Dudarev formalism [3]. The exchange parameters for a Heisenberg Hamiltonian were then derived with the TB2J Python package [4] by downfolding the DFT bands in the vicinity of the Fermi energy employing Wannier functions.
First, we studied $CrPS_4$ and found an FM ground state with a magnetic moment of 3.0 μB/magnetic atom, in agreement with the literature [5]. The exchange parameters of $CrPS_4$ were analyzed in detail, providing insight into the competition between different exchange-interaction mechanisms.



Second, we compared the exchange interaction in $CrPS_4$ and $NiPS_3$. For NiPS3, our results showed that the essential interaction is the AFM superexchange with the third neighbor, which overcomes all the others because of the alignment of sulfur atoms in a plane that offers a favored path for the interaction, which is in agreement with previous studies [5].

In summary, our comprehensive study of $CrPS_4$ provides a deeper understanding of why $CrPS_4$ exhibits FM order. This insight opens up possibilities for targeted modification of $CrPS_4$'s magnetic properties, a significant step forward in materials science and condensed matter physics.

References:

1. R. Samal et al. J. Mater. Chem. A, 9 2560-2591 (2021).
2. Peng et al. m Advanced Materials, 32 2001200 (2020).
3. Dudarev et al., Physical Review B, 57 1505–1509 (1998).
4. He et al. C. Computer Physics Communications, 264 107938 (2021).
5. Wu et al., RSC Advance, 9 30655–30658 (2019).

Acknowledgement of financial support: We would like to thank the German Science Foundation (DFG) for supporting this work with the DIP grant No.1223-21. And, also acknowledges the financial support by the DFG via the SFB 1415, Project ID No. 417590517.

Statistical approach to optimize production of lipopeptide biosurfactant by Pseudomonas fluorescens DSS73

Tomasz Janek[1], Mateusz Kruszelnicki[2], Martyna Romanowska[2], Izabela Polowczyk[2]

[1] *Wrocław University of Environmental and Life Sciences, Wrocław, Poland*

[2] *Wrocław University of Science and Technology, Wrocław, Poland*

271824@student.pwr.edu.pl, tomasz.janek@upwr.edu.pl, mateusz.kruszelnicki@pwr.edu.pl, izabela.polowczyk-@pwr.edu.pl

Several microorganisms are known to produce a wide variety of surface-active substances referred as biosurfactants. Most biosurfactants are obtained using costly culture media and purification processes, which limits their wider industrial use. The utilization of waste as a feedstock for production of value-added bioproducts has opened new avenues contributing to environmental sustainability. The main objective of this study is to optimize biosurfactant production by *Pseudomonas fluorescens* DSS73 with statistical approaches. Lipopeptide biosurfactant production from *P. fluorescens* DSS73 was carried out with different carbon sources, and maximum yield was achieved with waste glycerol, a raw material obtained from crude biodiesel production. The important medium components identified by the Plackett–Burman method were waste glycerol and urea along with culture parameter, cultivation time. Box–Behnken response surface methodology was applied to optimize biosurfactant production. The maximum estimated value of product yield on biomass growth (Yp/x) was 0.78 g/g. The obtained lipopeptide biosurfactant is able to reduce the surface tension of water up to 27 mN/m.

The obtained experimental results concludes that Box–Behnken designs are very effective statistical tools to improve biosurfactant production. These results may be useful to develop a high efficient production process of biosurfactant. In addition, this type of kinetic modeling approach may constitute a useful tool to design and scaling-up of bioreactors for the production of biosurfactant.

References:

Acknowledgement of financial support: This work was financed by the National Science Centre, Poland, OPUS-24 grant No. 2022/47/B/ST8/03392, project title: "Study of novel lipopeptide biosurfactants effect on the stability of a thin liquid film and the formation of a three-phase contact in terms of their use in flotation".

Computer methods for detection and analysis of displacement of breast cancer lesions

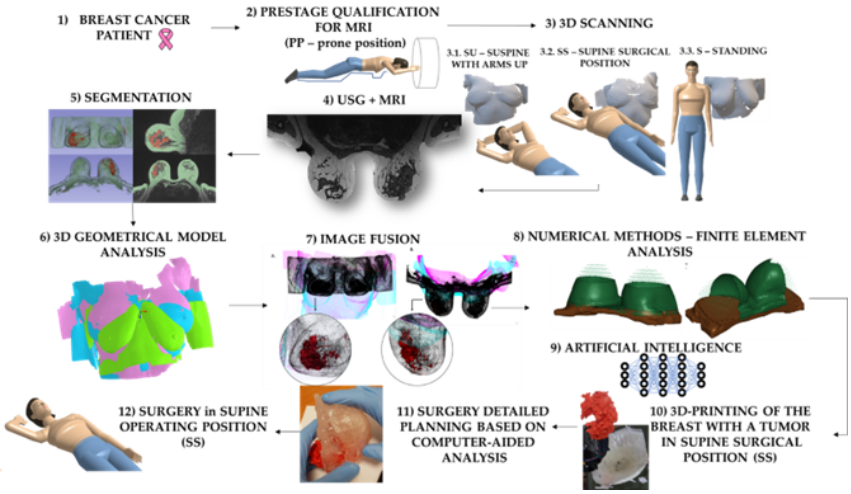
Adrianna Szumiejko[1], Bartosz Dołęga-Kozierowski[2], Mariusz Ptak[1]

[1] *Wrocław University of Science and Technology, Wrocław, Poland*

[2] *Dolnośląskie Centrum Onkologii, Pulmonologii i Hematologii, Wrocław, Poland*

adrianna.szumiejko@pwr.edu.pl, mariusz.ptak@pwr.edu.pl

This research addresses the challenge of precisely locating breast tumors during MRI scans, which affects how surgeries are planned. It outlines a methodological process that combines pre-qualification assessments, 3D scans, MRI, and USG imaging, along with segmentation and finite element analysis. An artificial neural network helps predict tumor movement, aiding in creating detailed surgical plans and 3D-printed breast models. This comprehensive approach, utilizing techniques like image fusion and additive manufacturing, allows for precise planning of lumpectomy surgery in the supine position. The study demonstrates significant potential in enhancing surgical accuracy and effectiveness for breast cancer patients, aiding in pathomorphological justification and improving preoperative planning. Transparent 3D-printed breast models serve as valuable tools for surgeons to visualize tumors more accurately.



References:

Acknowledgement of financial support:

Lanthanide-Activated Nanoparticles: Application for Personalized Cancer Treatment and Temperature Control of Cancer Cells

Dominika Grzesiak[1], Eugeniusz Zych [1], Justyna Zeler[1]

[1] *University of Wrocław, Wrocław, Poland*

eugeniusz.zych@uwr.edu.pl, 340666@uwr.edu.pl, justyna.zeler@uwr.edu.pl

The project focuses on exploring an optically active nanomaterial based on perovskites triply-doped with Cr^{3+} and thoughtfully selected Ln^{3+} ions (Ln(1)=Sm, Eu, Yb and Ln(2)=Er) with near-infrared (NIR) afterglow emission and persistent luminescence thermometry properties. The research aims to uncover potential application of such materials in theranostic approaches to biomedicine. These materials are synthesized for diagnostic purposes and utilize their thermoluminescent (TL) capability to concurrently measure the temperature of specific cells or organelles during targeted cancer treatment. Such temperature monitoring under physiological conditions could offer valuable insights for controlling localized magnetic or optical hyperthermia effects.

Additionally, the project conducts comprehensive photoluminescence measurements, including absolute quantum yield emission (QY) at room temperature, along with photoluminescence (PL), photoluminescence excitation (PLE), and emission decay curves (DEC) generated by various dopants. These detailed analyses offer crucial insights into the material's behavior and performance within the physiological temperature range, crucial for advancing its potential biomedical applications. The findings will be shared at a poster presentation for comprehensive in-depth discussion.

References:

Acknowledgement of financial support: The research finances by the Polish National Science Centre under OPUS grant UMO-2023/49/B/ST5/04265.

Discovery of the complex behavior of biological membrane domains in cells and model membrane systems

Aleksander Czogalla[1], Agnieszka Biernatowska[1], Dominik Drabik[1], Karolina Wójtowicz[1]

[1] *University of Wrocław, Wrocław, Poland*

aleksander.czogalla@uwr.edu.pl

Biological membranes are known for their complexity, with the formation of membrane domains, such as membrane rafts, being of central importance for the successful execution of various cellular processes. However, due to their nanoscale properties, these domains are often understudied as the experimental techniques required for their quantitative investigation are challenging. To address this issue, we have utilized both super resolution imaging and advanced biophysical approaches such as fluorescence lifetime imaging microscopy (FLIM) and spot-variation fluorescence correlation spectroscopy (svFCS) to study rafts in cell membranes and model membrane systems. We demonstrated that some peripheral proteins act as key raft-capturing molecules that regulate the temporal immobilization of membrane nanoclusters and control the local concentration and confinement of membrane raft makers. We also developed an original methodological approach combining confocal microscopy, svFCS and Z-scan approach together with giant unilamellar vesicles (GUVs) to obtain quantitative data on the behavior of signaling lipids in free-standing membranes. Not only did we succeed in comprehensively describing the dynamics and domain formation of these lipids at the nano- and microscale, but also in demonstrating that minute differences in their structure strongly influence the behavior of these lipids. Importantly, the experimental approach we have developed opens up new possibilities in membrane biophysics, as it can be used to study other molecules embedded in the membrane.

References:

Acknowledgement of financial support: This work was possible thanks to the financial support from the National Science Centre (Poland) grant no 2018/30/E/NZ1/00099.

Towards electronic microplates with multimodal sensing for bioassays

Daniel Nieder[1], Isli Cela[1], Larysa Baraban[1], Zeljko Janicijevic[1]

[1] *Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany*

z.janicijevic@hzdr.de, l.baraban@hzdr.de, d.nieder@hzdr.de

Scientists and clinicians across various disciplines rely on the use of microplates in laboratories and clinical settings. Traditional optical measurement techniques involving cumbersome microplate readers and advanced microscopes offer valuable insights into biological systems. These techniques typically require trained personnel, often limiting their use to dedicated core laboratories. In addition, many bioassays require staining, which increases complexity, and sample processing times. We introduce a novel thermal-based readout method that offers a cost-effective, user-friendly, and real-time alternative to complement the traditional strategies. This new approach has the potential to broaden the accessibility and simplify the bioassay analysis.

Thermal sensors can be seamlessly integrated into standardized microplate formats. The sensing principle relies on the inversely proportional relationship between resistance change and heating power, generated through Joule heating. The so-called modified Transient Plane Source technique is sensitive to changes in the thermal effusivity of the sample, which can be related to changes in biological properties. Additionally, by precisely controlling the power between measurement pulses, we gain the capability to control baseline temperature, providing both incubation and sensing functions with a single thermal element. This added versatility enhances the potential applications of thermal-based readouts in various bioassays. We aim to demonstrate our proof-of-concept using a straightforward and reliable biological system tracking bacterial growth. Yet, our approach extends beyond the integration of thermal sensors into microplates. Our device will be driven by low-power microcontroller-based Arduino UNO R4 WiFi electronics, enabling smartphone controlling, wireless data transmission, and cloud-based storage. The overarching vision is to create a versatile multimodal sensing interface capable of not only controlling the environment but also measuring a range of factors, including thermal bulk properties, electrical bulk properties, and specific biomarkers.

References:

Acknowledgement of financial support:

Bayesian Parameter Estimation for Relativistic Heavy-Ion Collisions: Phenomenology of Identified Particle Spectra

Oleksandr Vitiuk[1], Benjamin Dönigus[2], David Blaschke[1], Gerd Roepke[3]

[1] *University of Wrocław, Wrocław, Poland*

[2] *Johann-Wolfgang-Goethe University, Frankfurt, Germany*

[3] *Universität Rostock, Rostock, Germany*

d.blaschke@hzdr.de, oleksandr.vitiuk@cern.ch

The Zubarev approach of the non-equilibrium statistical operator [1] is used to account for the enhancement of the low-protect p_T part of pion spectra by introducing an effective pion chemical potential [2]. This is an alternative to the explanation of the low-protect p_T enhancement by resonance decays. We report on the first results obtained with a newly developed thermal particle generator that implements both mechanisms of low-protect p_T enhancement. With the help of the principal component analysis and Gaussian processes emulators based surrogate model, Bayesian inference methods were applied for these scenarios to find the most probable sets of thermodynamic parameters at the freeze-out hypersurface for the case of the transverse momentum spectra of identified particles measured by the ALICE Collaboration.

References:

1. D.N. Zubarev et al., Statistical Mechanics of Nonequilibrium Processes, Akademie Verlag Berlin (1996), vol. I.
2. D. Blaschke et al., Particles 3, 380–393 (2020).

Acknowledgement of financial support: We acknowledge support by NCN under grant No. 2021/43/P/-ST2/03319 (D.B.) and grant No. 2022/45/N/ST2/02391 (O.V.). The work of G.R. was supported via a joint stipend from the Alexander von Humboldt Foundation and the Foundation for Polish Science.

Statistical approach to optimize production of lipopeptide biosurfactant by Pseudomonas fluorescens DSS73

Izabela Polowczyk[1], Tomasz Janek[2], Mateusz Kruszelnicki[1], Martyna Romanowska[1]

[1] *Wrocław University of Science and Technology, Wrocław, Poland*

[2] *Wrocław University of Environmental and Life Sciences, Wrocław, Poland*

271824@student.pwr.edu.pl, tomasz.janek@upwr.edu.pl, mateusz.kruszelnicki@pwr.edu.pl, izabela.polowczyk@pwr.edu.pl

Several microorganisms are known to produce a wide variety of surface-active substances referred as biosurfactants. Most biosurfactants are obtained using costly culture media and purification processes, which limits their wider industrial use. The utilization of waste as a feedstock for production of value-added bioproducts has opened new avenues contributing to environmental sustainability. The main objective of this study is to optimize biosurfactant production by *Pseudomonas fluorescens* DSS73 with statistical approaches. Lipopeptide biosurfactant production from *P. fluorescens* DSS73 was carried out with different carbon sources, and maximum yield was achieved with waste glycerol, a raw material obtained from crude biodiesel production. The important medium components identified by the Plackett–Burman method were waste glycerol and urea along with culture parameter, cultivation time. Box–Behnken response surface methodology was applied to optimize biosurfactant production. The maximum estimated value of product yield on biomass growth (Yp/x) was 0.78 g/g. The obtained lipopeptide biosurfactant is able to reduce the surface tension of water up to 27 mN/m.

The obtained experimental results concludes that Box–Behnken designs are very effective statistical tools to improve biosurfactant production. These results may be useful to develop a high efficient production process of biosurfactant. In addition, this type of kinetic modeling approach may constitute a useful tool to design and scaling-up of bioreactors for the production of biosurfactant.

References:

Acknowledgement of financial support: This work was financed by the National Science Centre, Poland, OPUS-24 grant No. 2022/47/B/ST8/03392, project title: "Study of novel lipopeptide biosurfactants effect on the stability of a thin liquid film and the formation of a three-phase contact in terms of their use in flotation".

Governing Energy Storage Capabilities via Dual Photo- and Thermal Stimulation in Lu_2O_3:Tb,M (M=Ti, Hf)

Dagmara Kulesza[1], Eugeniusz Zych[1]

[1] *University of Wrocław, Wrocław, Poland*

dagmara.kulesza@uwr.edu.pl, eugeniusz.zych@uwr.edu.pl

The ability of inorganic phosphors to store energy from previous exposure to high-energy radiation, gamma- or X-rays, UV radiation, or sunlight has puzzled scientists for years. Understanding the phenomenon of energy storage itself is an even greater challenge. The key to unlocking this mystery lies in tracing the migration of free electrons and holes after the irradiation, along with their capture at specific levels of charge traps. It is also important to analyze their locations among the energy levels of the matrix and the activators used.

Understanding the mechanisms governing such phenomena proved to change between materials and is crucial due to the existing and potential applications of these materials. They can be used in various gadgets, specialized lighting (such as evacuation routes, bicycle paths, and road signs), medical imaging, or dosimetry [1].

The study that has been presented provides a fresh perspective on the trapping of excited charges in Lu_2O_3:Tb,M (M= Ti, Hf) ceramics, uncovering their unique characteristics as storage and/or persistent luminescence phosphors [2]. The research uses a range of experiments, rooted in thermoluminescence and thermoluminescence excitation spectroscopy, to reveal the dual nature of these materials. The focus of the study is on the Lu2O3:Tb,Ti system, which can efficiently produce persistent luminescence due to the presence of shallow traps that can only be charged under specific irradiation conditions with 360 nm light. Moreover, the study shows that altering the sample charging, temperature significantly affects the efficiency of trap filling – both shallow (at room temperature) and deeper (at higher temperatures). These findings are a significant contribution to the field and demonstrate the potential for Lu_2O_3:Tb,M (M= Ti, Hf) ceramics to be used as efficient and stable persistent luminescence phosphors.

References:

1. P.F. Smet, K. Van den Eeckhout, O.Q. De Clercq, D. Poelman, Handbook on the Physics and Chemistry of Rare Earths, Vol. 48 92015) Chapter 274, 1-108.
2. D. Kulesza, A.J.J. Bos, E. Zych, Acta Materialia, 231 (2022), 117852/1-117852/9.

Acknowledgement of financial support: Research project partly supported by program "Excellence Initiative – Research University" (IDUB) for years 2020-2026 for University of Wrocław (grant # BPIDUB.4610.21.2021.KP.B).

Holistic recovery of recyclable materials from Waelz slag

Junnile Romero[1], Ajay Patil[1], Alexandros Charitos[2], Ari Vaisanen[3], Henrik Funke[4], Ludwig Blenau[2], Norman Kelly[1], Sandra Gelbrich[4], Volker Recksiek[1]

[1] *Helmholtz Institute Freiberg for Resource Technology (HIF), Freiberg, Germany*

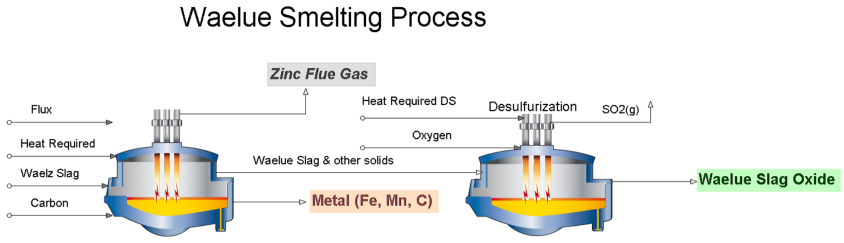
[2] *Technische Universität Bergakademie Freiberg (TUBAF, Freiberg, Germany*

[3] *The University of Jyväskylä, Jyväskylä, Finland*

[4] *Steinbeis Innovation Center FiberCrete gGmbH, Chemnitz, Germany*

j.romero@hzdr.de

Different industries consumes zinc (Zn), such as battery, cosmetics, pharmaceuticals, and metals. Due to urbanization and technological advancement, the need for efficient resource management of Zn is necessary. The most widely used Zn containing scrap recycling method is the Waelz process, particularly for electric arc furnace dust (EAFD). Approximately, the world's annual production of EAFD is 7.5 million tons with which 45% is recycled. By effectively recovering Zn from such waste using the principles of resource efficiency and circularity, offers a sustainable solution to address the escalating demand for Zn while mitigating the environmental burdens.



Waelz Process is a pyro metallurgical technique where the Zn scrap is loaded into a rotary kiln together with a carbon-containing reducing agent at 1200-1300 oC to extract Zn. The airflow limits the penetration of oxygen from the reaction environment into the material bed. Coke and CO (products of partial carbon oxidation) convert ZnO and Zn ferrite to Zn metal. Zn is vaporize and oxidizes in the gas stream to form ZnO, which is collected on bag filters. In Europe, the Zn recovered through this process is approximately 250,000 tons/year and the slag generated is nearly 800,000 tons/year called "Waelz Slag". However, similar to other slags further utilization of Waelz slag is a problem due to the lack of environmental compatibility, especially because of the complex chemical and mineralogical composition, as a result, Waelz slag is largely landfilled, even though the iron content exceeds that of high-grade iron ores. Through a new smelting reduction method in a high-temperature furnace similar to the study previous studies, this initiative intends to revolutionize Waelz slag recycling. The project hope to overcome the limits of old approaches by adopting this innovative technique, it allows to realize the full potential of Waelz slag as a valuable

resource.

References:

Acknowledgement of financial support:

Siderophore assisted recycling of gallium and germanium from their low concentrated wastewaters

Aratrika Ghosh[1], Rohan Jain,[1], Katrin Pollmann[1]

[1] *Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany*

r.jain@hzdr.de, a.ghosh@hzdr.de, k.pollmann@hzdr.de

Critical metals like gallium (Ga) and germanium (Ge) hold strategic importance in the development of modern technologies like optoelectronic devices, semiconductors, transistors, light-emitting diodes, and many more[1,2]. The supply of these metals is not assured due to many reasons. Therefore, new sources and efficient recovery techniques need to be identified. Thus, attention should be drawn to sources with very low concentrations of these metals which are usually neglected. The reason for such negligence is the presence of high concentrations of contaminant metals and very low concentrations of these critical metals. Thus, a highly specific, selective, economical, and sustainable process is needed to recover and recycle these metals.

Siderophore assisted technology "GaLIophore" could be a one-point solution. In GaLIophore siderophore Desferroxamine B (DFOB) was used to selectively adsorb Ga from industrial wastewater[3]. DFOB is a highly selective molecule that forms a highly stable complex with Ga in an equimolar stoichiometric ratio. It was seen that the complexation of Ga with DFOB was independent of pH and background electrolyte. This technology was then extended to Ge and the complexation of Ge with DFOB was studied. However, with Ge, it was seen that complexation was preferred in acidic pH and was also affected by high-concentration anions like chloride. Moreover, to make the technology economical and sustainable, DFOB was re-generated by the addition of non-specific ligand ethylenediaminetetraacetic acid (EDTA). More than 90% of DFOB were re-generated by the addition of 6 times and 8 times excess of EDTA at pH of 3.5 for Ga and Ge respectively. This led to the recovery of more than 90% for both metals with DFOB complexation at the end of the process. Thus, this technology for the first time demonstrated a solution to recycling these critical metals from low concentrated systems in a sustainable and eco-friendly manner.

References:

1. Patel, M.; Karamalidis, A. K. Germanium: A Review of Its US Demand, Uses, Resources, Chemistry, and Separation Technologies. Separation and Purification Technology. Elsevier B.V. November 15, 2021. https://doi.org/10.1016/j.seppur.2021.118981.
2. Saikia, S.; Costa, R. B.; Sinharoy, A.; Cunha, M. P.; Zaiat, M.; Lens, P. N. L. Selective Removal and Recovery of Gallium and Germanium from Synthetic Zinc Refinery Residues Using Biosorption and Bioprecipitation. J Environ Manage 2022, 317. https://doi.org/10.1016/j.jenvman.2022.115396.

3. Jain, R.; Fan, S.; Kaden, P.; Tsushima, S.; Foerstendorf, H.; Barthen, R.; Lehmann, F.; Pollmann, K. Recovery of Gallium from Wafer Fabrication Industry Wastewaters by Desferrioxamine B and E Using Reversed-Phase Chromatography Approach. Water Res 2019, 158, 203–212. https://doi.org/10.1016/-j.watres.2019.04.005.

Acknowledgement of financial support:

Recognition of NeuGc GM3 ganglioside by the anti-tumor antibody 14F7 is modulated by the membrane environment.

Michał Grzybek[1]

[1] *Technische Universität Dresden, Dresden, Germany*

michal.grzybek@tu-dresden.de

Aberrant glycosylation is a common feature related to tumor progression, making tumor-associated glycolipids promising molecular targets in antineoplastic therapies and vaccine strategies. 14F7 is an anti-tumor antibody with high clinical potential, which has an extraordinary specificity for NeuGc GM3, but does not recognize the very similar, ubiquitous NeuAc GM3. Understanding the molecular details of this specificity would highly reinforce the value of 14F7 as a novel anti-cancer drug. Using model membrane systems, we show that 14F7 recognizes NeuGc GM3 only above a certain threshold of lipid concentrations. This "all-or-nothing" effect was exacerbated in giant unilamellar vesicles and multilamellar vesicles, whereas no binding was observed to 100 nm liposomes, emphasizing that the 14F7–NeuGc GM3 interaction is additionally modulated by membrane curvature. Unexpectedly, the presence of other glycolipids in the membranes strongly modulated the binding affinity to NeuGc GM3-containing liposomes. This effect may be important for tumor recognition, where the overall changes in glycolipid profiles may enhance 14F7 binding to even small amounts of NeuGc GM3.

References:

Acknowledgement of financial support:

New Approaches to Raman spectra analysis

Simon Liebing[1], Oliver Heymer[1], Paul Feiler[1], Simon Brehm[1], Jens Kortus[1]

[1] *Technische Universität Bergakademie Freiberg, Freiberg, Germany*

simon.liebing@physik.tu-freiberg.de

PyRamanGUI[1, 2, 3] is a versatile tool to analyze Raman spectra, which combines state-of-the-art analysis methods like baseline correction, smoothing, cosmic spike removal, peak fitting and multivariate statistical methods like principal compound analysis with the organization of Raman data in projects and the plotting of spectra. The automated evaluation of batches of Raman spectra is also available.
The projects allow to store additional information on experimental details and samples together with the data, plots and evaluated Raman spectra. The program is constructed as a graphical user interface, so no knowledge in coding is required for its use. The source code is completely written in Python and freely available (https://gitlab.com/brehmsi/PyRamanGUI).
In a next step we want to improve on automatic identification of Raman bands using information from databases of Raman spectra. One idea for future development is to implement a neural network that can suggest possible materials or material combinations matching an experimental Raman spectra from an unknown material.

References:

1. GitLab repository mit dem Code: https://gitlab.com/brehmsi/PyRamanGUI.
2. S. Brehm, C. Himcinschi, J. Kraus, J. Kortus, SoftwareX, 23, 101486, 2023, https://doi.org/10.1016/-j.softx.2023.101486.
3. Simon Brehm, Dissertation 2023 https://nbn-resolving.org/urn:nbn:de:bsz:105-qucosa2-884021.

Acknowledgement of financial support:

Electronic Lieb lattice signatures embedded in two-dimensional polymers with square lattice

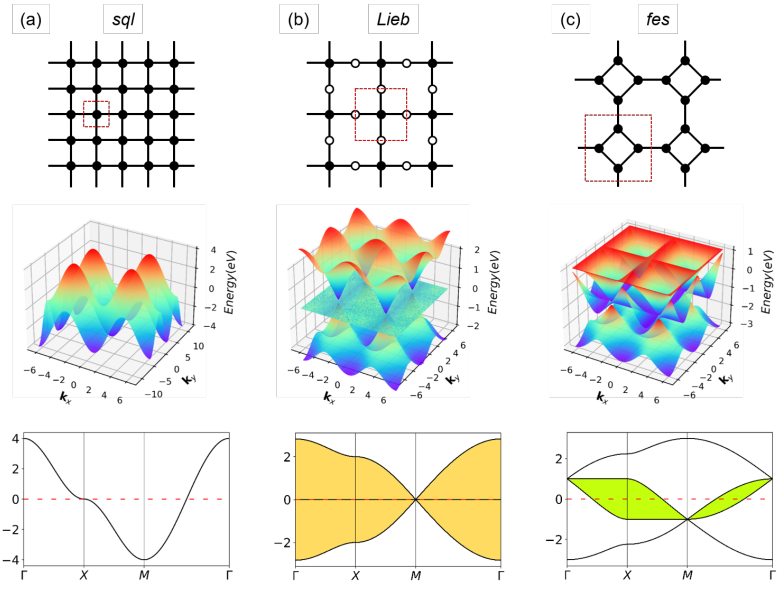
Yingying Zhang[1], Miroslav Položij[1,2], Shuangjie Zhao[2], Thomas Heine[1,2]

[1] *Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Center for Advanced Systems Understanding (CASUS), Görlitz, Germany*

[2] *Technische Universität Dresden, Dresden, Germany*

miroslav.polozij@tu-dresden.de, shuangjie.zhao@tu-dresden.de, yingying.zhang@hzdr.de, thomas.heine@tu-dresden.de

Exotic band features, such as Dirac cones and flat bands, arise directly from the lattice symmetry of materials. The Lieb lattice is one of the most intriguing topologies, because it possesses both Dirac cones and flat bands which intersect at the Fermi level. However, the synthesis of Lieb lattice materials remains challenging. Here, we explore two-dimensional polymers (2DPs) derived from zinc-phthalocyanine (ZnPc) building blocks with a square lattice (sql) as potential electronic Lieb lattice materials. By systematically varying the linker lengths (ZnPc-xP), we found that some ZnPc-xP exhibit a characteristic Lieb lattice band structure. Interestingly though, fes bands are also observed in ZnPc-xP. The coexistence of fes and Lieb in sql 2DPs challenges the conventional perception of the structure-electronic structure relation. In addition, we show that manipulation of the Fermi level, achieved by electron removal or atom substitution, effectively preserves the unique characteristics of Lieb bands. The Lieb Dirac bands of ZnPc-4P show Chern insulator states with non-zero Chern number. Our discoveries provide a fresh perspective on 2DPs and redefine the search for Lieb lattice materials into a well-defined chemical synthesis task.



References:

1. https://pubs.rsc.org/en/content/articlehtml/2024/sc/d3sc06367d

Acknowledgement of financial support:

Site-Selective Spectroscopy of $SrAl_{12}O_{19}$:Eu^{2+}, Eu^{3+}, Cr^{3+} Luminescence Thermometric Phosphors

Pola Łukaszczuk[1], Justyna Zeler[1], Małgorzata Sójka[1], Eugeniusz Zych[1]

[1] *University of Wrocław, Wrocław, Poland*

eugeniusz.zych@uwr.edu.pl, malgorzata.sojka@ge.com, 338803@uwr.edu.pl, justyna.zeler@uwr.edu.pl

This study presents the results of research on the photoluminescent properties of the inorganic phosphor $SrAl_{12}O_{19}$ doped with Eu^{2+}, Eu^{3+} and Cr^{3+}. The concentrations for Eu and Cr were 1mol%, respectively, with respect to Sr and Al. The research was focused on evaluating the potential of this material as a luminescent thermometer. A set of photoluminescent measurements, such as luminescent emission and excitation spectra supplemented with decay time measurements, were performed in the 12 – 1000 K range of temperatures. The experiments exposed that Eu was present as Eu^{2+} and Eu^{3+}, both of which contributed to luminescence. The latter produced its characteristic orange-red luminescence with main components about 590 and 610 nm, while the former generated emission around 400 nm. At low temperatures, it constituted narrow lines resulting from the 6P7/2-8S7/2 transition and broadband due to the 5d-4f luminescence. Cr^{3+} was found to generate emission around 700 nm, and detailed studies at 12 K proved that this dopant occupied at least three crystallographically different symmetry sites. This is in agreement with the structure of the host lattice.

Emission characteristics of the three luminescent centers were shown to change with temperature differently. Both the spectra and the decay times were temperature-dependent. The presentation will discuss the details and will seek the most promising thermometric parameters out of all available. The luminescence of this material is based on charge transfer, f-d, d-d transitions. The efficient absorption transitions of all three luminescent centers, Eu^{2+}, Eu^{3+} and Cr^{3+}, allow for efficient excitation of their emissions. This is an important advantage of any luminescent thermometer and makes the $SrAl_{12}O_{19}$ doped with Eu^{2+}, Eu^{3+} and Cr^{3+} additionally attractive for such applications.

References:

Acknowledgement of financial support: The Polish National Science Centre (NCN) financed the research under OPUS grant #2018/31/B/ST4/00924.

Advancing the biomedical applications of nanophosphors through the synergy of thermoluminescence and luminescent thermometry

Aleksandra Owczarek[1], Eugeniusz Zych[1], Justyna Zeler[1]

[1] *University of Wrocław, Wrocław, Poland*

eugeniusz.zych@uwr.edu.pl, justyna.zeler@uwr.edu.pl, 322286@uwr.edu.pl

Luminescent nanomaterials are becoming an increasingly fascinating area of research, especially considering their potential application in medicine, particularly in personalized cancer therapy projected to be the next giant step in the development of medicine.

Within the scope of this project, innovative luminescent nanomaterials will be developed, characterized by both, long-lasting luminescence and the ability for precise temperature measurement through the thermoluminescence effects. Our research will focus on synthesizing $LaAlO_3$ perovskite activated by Cr^{3+} ions. We are particularly interested in the influence of co-doping $LaAlO_3$:Cr with selected lanthanide ions. The project includes also their comprehensive physicochemical and spectroscopic characterization, as well as in-depth analysis of their temperature-dependent properties.

These materials have the potential for application in personalized cancer therapy through diagnostics and controlled hyperthermia generation. Detailed spectroscopic analysis under physiological temperature conditions will enable the utilization of these materials in optical imaging of tumor tissues and precise temperature measurement through temperature-dependent luminescence. The results of these studies are crucial for further development of personalized cancer therapy and medical diagnostics.

References:

Acknowledgement of financial support: The research finances by the Polish National Science Centre under OPUS grant UMO-2023/49/B/ST5/04265.

openPMD - the Open Standard for Particle-Mesh Data

Franz Poeschel[1]

[1] *Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Center for Advanced Systems Understanding (CASUS), Görlitz, Germany*

f.poeschel@hzdr.de

The Open Standard for Particle-Mesh Data (openPMD) is a F.A.I.R. metadata standard for tabular (particle/dataframe) and structured mesh data in science and engineering.
CASUS/HZDR is developing this data standard and its flagship implementation, the openPMD-api, in close collaboration with the Lawrence Berkeley National Laboratories and further open-source contributors.
This presentation gives an overview on codes that use openPMD. This includes in-house use where the standard is applied as the I/O solution for codes such as the particle-in-cell simulation PIConGPU or the density functional theory framework MALA. openPMD is further used within as well as outside the Helmholtz community, including many international codes.
CASUS and openPMD are part of the HELPMI project of the Helmholtz metadata collaboration, further tying the standard into the Helmholtz community in an explorative project to find a useful standard for Laser-Plasma experiments.
By implementing the data standard openPMD in various file standards from JSON over TOML and HDF5 to ADIOS2, the openPMD-api targets a range from simple prototyping workflows up to recent supercomputing systems, including recent full-scale runs on OLCF Frontier, the current TOP1 system in the world. This talk demonstrates how scientists can harness scalable I/O solutions on state-of-the-art systems without the mental overhead of writing low-level I/O routines.

References:

Acknowledgement of financial support:

Thermometric Phosphors – The Effect of Bandgap Engineering on Energy Storage After Exposure to X-rays

Paulina Bolek[1], Eugeniusz Zych[1]

[1] *University of Wrocław, Wrocław, Poland*

paulina.bolek@uwr.edu.pl, eugeniusz.zych@uwr.edu.pl

Thermoluminescence is light produced by heating a phosphor to a temperature below that of incandescence. The emission of light is only observed after earlier exposure of the phosphor to ionizing high-energy radiation, often X-rays, UV, or blue radiation. The heat only triggers the effect [1]. The main applications of thermoluminescent materials include radiation dosimetry (environmental, clinical/medical, and high-dose dosimetry), dating, temperature sensing, in-vivo bioimaging, or digital radiography.

Bandgap engineering is a tool used to modify and manage the properties of phosphors. It allows tailoring trap depths to enhance persistent luminescence duration and intensity as well as to reduce or remove an afterglow emission, usually a detrimental property of scintillators and photoluminescent phosphors. Bandgap modification can significantly affect the thermoluminescence properties of materials, as it allows managing trap depths, the crucial parameter of thermoluminescent phosphors.

Recently, we have proven that the bandgap engineering executed by changing the Al:Ga ratio in $Y_3(Al,Ga)_5O_{12}$:0.1%Pr phosphors significantly affects their photoluminescent properties and improves their thermometric parameters, making them high-quality dual-mode luminescence thermometers with a manageable range of the highest sensitivity [2].

In this presentation, we will show how bandgap modification in $Y_3(Al,Ga)_5O_{12}$:0.1%Pr affects their thermoluminescence. We shall show that all the phosphors exhibit intense thermoluminescence after exposure to X-rays. Selected phosphors of the series exhibit intense, persistent luminescence. The common feature of the presented materials is the recombination center, the Pr^{3+} ion. Yet, the spectra produced by the dopant depend significantly on the Al:Ga ratio. All these properties will be discussed in detail.

References:

1. A.J.J. Bos, Thermoluminescence as a research tool to investigate luminescence mechanisms, Materials (Basel). 10 (2017) 1–22.
2. P. Bolek, J. Zeler, C.D.S. Brites, J. Trojan-piegza, L.D. Carlos, E. Zych, Ga-modified YAG:Pr^{3+} dual-mode tunable luminescence thermometers, Chem. Eng. J. 421 (2021) 129764.

Acknowledgement of financial support: Research supported by program „Excellence initiative – research university" for years 2020-2026 for University of Wrocław.

Unveiling the Biomedical Potential of Luminescent Materials Exploring their Concerted Thermoluminescent and Thermometric Performance

Aleksandra Małoń[1], Eugeniusz Zych[1], Justyna Zeler[1]

[1] *University of Wrocław, Wrocław, Poland*

eugeniusz.zych@uwr.edu.pl, justyna.zeler@uwr.edu.pl, 322261@uwr.edu.pl

Luminescent thermometers exhibiting also thermoluminescence effect are of great interest in various fields including chemistry, biology, and medicine. They have significant potential as effective tools, particularly in optical imaging of tumor tissues and simultaneous temperature readings with the spatial resolution at the level of single cells.

Promising compounds demonstrating both thermoluminescence and luminescence thermometry effects are triple-doped perovskites with lanthanum aluminate as the matrix. They are activated with Cr^{3+} ions and chosen lanthanide ions, for example Sm^{3+} and Ho^{3+}. Research on these materials focuses on their ability to simultaneously exhibit two physical phenomena: near-infrared (NIR) afterglow emission and the read-out of the temperature through the thermoluminescence. Combination of such effects and their control show potential for simultaneous cancer cells imaging and overheating them to death by means of controlled luminescence effects.

The project is at its very early stage. Synthesized materials will be characterized for their phase purity (XRD), IR spectroscopy, and morphology (SEM/TEM). Standard optical measurements at room temperature (emission spectra (PL), excitation spectra (PLE), and time-resolved luminescence dynamics of activators) will also be performed to recognize the phosphors capabilities. The results of the above studies will be presented at a poster presentation.

References:

Acknowledgement of financial support: The research finances by the Polish National Science Centre under OPUS grant UMO-2023/49/B/ST5/04265.

Employing The Chou-Talalay method and CompuSyn software to analyze synergism between phenethyl isothiocyanate and anti-cancer agents

Ewa Olczak[1], Jerzy Gubernator[1]

[1] *University of Wrocław, Wrocław, Poland*

ewa.olczak@uwr.edu.pl, jerzy.gubernator@uwr.edu.pl

The Chou-Talalay method and CompuSyn software are tools used in drug combination studies. The Chou-Talalay method employs mathematical models to establish dose-effect relationships and analyze drug interactions, while CompuSyn uses that theory for automated calculation of Combination Index. Combination Index below 1 indicates synergism, equal 1 indicates additive effect and above 1 indicates antagonism. This approach allows to easily establish promising drug combinations *in vitro*. Various drug combinations are utilized to achieve better outcomes in patients, particularly those suffering from malignant tumors. Combining different anti-cancer agents enhance treatment efficacy, help overcome drug resistance and minimize adverse effects.

By employing The Chou-Talalay method and CompuSyn software we analyzed interactions between phenethyl isothiocyanate (PEITC) and anti-cancer agents in two pancreatic cancer cell lines (BxPC-3 and AsPC-1). In the present study, we combined PEITC with one of the following compounds: gemcitabine, 5-fluorouracil, doxorubicin, cisplatin, oxaliplatin and determined cell growth inhibition with The Sulforhodamine B Cytotoxicity Assay. These data were entered into the CompuSyn software and Combination Index was calculated. The results of our study show that PEITC in certain concentrations exhibited synergistic outcomes (CI<1) with mentioned drugs. Further research will focus on examining the mechanism of action of these synergistic pairs.

References:

Acknowledgement of financial support:

Advancing animal movement modelling through the integration of human mobility science

Kamil Smolak[1], Adrian Kaczmarek[1], Alicja Kowalczyk[1], Anna Shepel[1], Grzegorz Jóźków[1], Jan Sierny[1], Krzysztof Hulewicz[1], Mieczysław Łyskawa[1], Przemysław Cwynar[1], Witold Rohm[1]; Wojciech Pusz[1], Wojciech Sowa[1]

[1] *Wrocław University of Environmental and Life Sciences, Wrocław, Poland*

kamil.smolak@upwr.edu.pl

The Integrated Science of Movement is a concept of a new field of study emerging from two very similar, yet independently and parallelly developing research areas, human mobility and movement ecology. The resulting combination is very interdisciplinary, combining knowledge and methods from GIScience, computer science, physics, geography, transportation, and public health. Thanks to the fast increase in the amount of collected massive datasets on the movement of humans, human mobility science developed rapidly, resulting in sophisticated algorithms and models dedicated to simulation studies. One of the goals of the Integrated Science of Movement is to transfer these developments to animal mobility, delivering unprecedented innovations to this area. This project explores the transferability of one of the most important discoveries of human mobility science, which is the universal and ubiquitous laws of movement. These laws are the foundation for human mobility simulation studies, which found their application in a vast range of areas, such as disaster response, traffic management and disease spread modelling. In the project, we gather high-quality spatiotemporal data on the movement of various species with the intent to develop the first-ever animal mobility model. The outcomes of this project will be integrated with an advanced disease spread prediction simulation designed for the prevention and mitigation of African Swine Fever (ASF) virus spread.

References:

1. Demšar, U., Long, J. A., Benitez-Paez, F., Brum Bastos, V., Marion, S., Martin, G., Sekulić, S., Smolak, K., Zein, B., & Siła-Nowicka, K. (2021). Establishing the integrated science of movement: bringing together concepts and methods from animal and human movement analysis. In International Journal of Geographical Information Science (Vol. 35, Issue 7, pp. 1273–1308). Taylor and Francis Ltd. doi: 10.1080/13658816.2021.1880589

Acknowledgement of financial support: Scientific work carried out by VERUS - Association of Producers of the Agricultural and Food Sector, co-financed from the state budget, under the program of the Minister of Education and Science called "Science for Society II", co-financing 1 960 185 PLN, total project value 1 960 185 PLN.

Interactions between SARS-CoV-2 spike fragment and ACE2-derived peptides or peptide-decorated liposomes

Aleksandra Kaczorowska[1], Mateusz Rzycki[2], Olga Michel[1], Aleksander F. Sikorski[3], Aleksander Czogalla[1]

[1] *University of Wrocław, Wrocław, Poland*

[2] *Wrocław University of Science and Technology, Wrocław, Poland*

[3] *Acellmed Ltd., Zabrze, Poland*

mateusz.rzycki@pwr.edu.pl, olga.michel@uwr.edu.pl, aleksandra.kaczorowska@uwr.edu.pl, aleksander.czogalla@uwr.edu.pl, aleksander.sikorski@uwr.edu.pl

The severe acute respiratory syndrome coronavirus type 2 (SARS-CoV-2), which causes the coronavirus disease 2019 (COVID-19) still poses a real threat to human health and challenges worldwide healthcare systems. Despite numerous mutations in the spike of SARS-CoV-2, which raise concerns about escape from vaccines and therapeutic drugs, the essential mechanism for virus infection remains unchanged – the viral spike protein binds to the angiotensin-converting enzyme II (ACE2). One of the strategies to inhibit the SARS-CoV-2 infection is a neutralisation of the virus before it enters human cells.

In our project, we explored the interactions of ACE2-derived peptides with the spike receptor binding domain (S-RBD) of SARS-CoV-2. Interaction studies between peptides and S-RBD were performed in silico and with microscale thermophoresis (MST). Based on molecular dynamics studies binding energies of several peptides and S-RBD were calculated. MST experiments revealed significant differences in the half-maximal effective concentration (EC50) of peptides. Two of the designed peptides were used in further experiments. Peptide-decorated liposomes were synthesized with the use of the selected peptides and then studies of their interactions with S-RBD were performed. Based on the results of MST studies we concluded, that the synthesized peptide-decorated liposomes interact with S-RBD and may be potentially used as SARS-CoV-2 inhibitors.

Our studies demonstrate, that ACE2-derived peptides and peptide-decorated liposomes interact with S-RBD, which shows their possible application as new anti-SARS-CoV-2 agents. Nanotherapeutics based on the structure of naturally occurring proteins seem a promising tool in a devising of novel antiviral strategies.

References: **Acknowledgement of financial support**: This Project “Mutation-resistant nano therapeutics inhibiting infection progress of RNA-virus, SARS-CoV-2” (2021/ABM/05/00002-00) is co-financed by the Medical Research Agency (Poland). It is conducted by the Polish Consortium of Acellmed Ltd., the Silesian Park of Medical Technology Kardio-Med Silesia, and the University of Wrocław.

Robust computational approach for including host-guest interactions in vibrational spectra of layered framework materials

Ekin Esme Bas[1], Karen Marlenne Garcia Alvarez[2], Andreas Schneemann[2], Thomas Heine[1,2], Dorothea Golze[2]

[1] *Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Center for Advanced Systems Understanding (CASUS), Görlitz, Germany*

[2] *Technische Universität Dresden, Dresden, Germany*

dorothea.golze@tu-dresden.de, thomas.heine@tu-dresden.de, e.bas@hzdr.de

We present a robust computational method to calculate vibrational spectra for two-dimensional framework materials, specifically for covalent-organic frameworks (COFs). Conventional methods like harmonic approximation fails to capture anharmonic modes and solvent bands which are often observed in the vibrational spectra of these materials. In this study, we employ an AIMD (ab initio molecular dynamics) based approach where we compute the IR and Raman intensities from the time-correlation functions of dipole moments and polarizabilities,[1] which aids us in the investigation of host-guest interactions. We present the AIMD-based IR and Raman spectra of COF-1 with and without 1,4-dioxane solvent molecules inside the pores. We dissect the obtained spectra into contributions coming from individual molecular units and solvent molecules in order to facilitate assignment of the peaks. Moreover, we explore the influence of different methods for calculating dipole moments and polarizability tensors on the IR and Raman intensities. We compare our AIMD-based spectra with the experimental data, and we show that our results reach an excellent agreement with experiment.

References:

1. M. Thomas, M. Brehm, R. Fligg, P. Voehringer, and B. Kirchner. Computing vibrational spectra from ab initio molecular dynamics. Phys. Chem. Chem. Phys. 2013, 15, 6608–6622.

Acknowledgement of financial support: We thank the German Research Foundation for support within the CRC 1415. We also acknowledge the Emmy Noether Programme of the German Research Foundation (project number 453275048) for funding.

Seed mucilaginous envelope - natural composite hydrogel

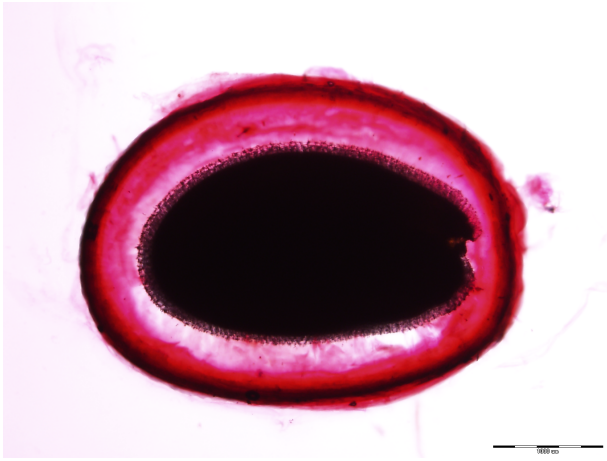
Agnieszka Kreitschitz[1], Alexander Kovalev[2], Eberhard Haase[2], Stanislav Gorb[2]

[1] *University of Wrocław, Wrocław, Poland*

[2] *Kiel University, Kiel, Germany*

akovalev@zoologie.uni-kiel.de, agnieszka.kreitschitz@uwr.edu.pl, sgorb@zoologie.uni-kiel.de, euahaase@gmx.de

The definition of hydrogel describes it as hydrophilic, three-dimensional, polymeric network able to absorb huge amount of water. Mucilage envelope produced by diverse plant seeds/fruits (diaspores) is considered as natural hydrogel and shares with it some specific features i.e. it is built of different polysaccharides (pectins, hemicelluloses and cellulose), which interact with each other via diverse types of bonds and form a three- dimensional network. Mucilage envelope due to the presence of hydrophilic pectins/hemicelluloses has an ability to absorb water. This aptitude to water absorption and gathering defines also the ecological role and the physical properties of the mucilage. First, the mucilage envelope creates the proper conditions for seed germination. In a fully hydrated stage mucilage demonstrates also very low frictional properties which play important role in seed dispersal via endozoochory. Second, water loss from the mucilage causes good adhe- sive properties, which are responsible for the diaspores attachment to the ground –anti-dispersal function or to the animals'body-epizoochoric dispersal. From industrial point of view, low friction and high adhesion are the properties that are essential in the medicine, bioengineering, cosmetics, food or pharmacy. Natural polymers, like seed mucilage, are most attractive source among diverse hydrogels particularly due to their high biodegradability, non-toxicity and non-irritability.



References:

Acknowledgement of financial support:

Molecular analysis of exon 21 of the TCOF1 gene in patients with Treacher Collins Syndrome unveiled a novel single nucleotide polymorphism.

Hubert Kokoszka[1], Bożena Marszałek-Kruk[1]

[1] *Department of Genetics, Wrocław University of Environmental and Life Sciences, Wrocław, Poland*

126306@student.upwr.edu.pl, bozena.marszalek-kruk@upwr.edu.pl

Treacher Collins syndrome (TCS) is a genetic disorder that affects the physical traits of mandibulofacial features. In patients with TCS the development of craniofacial bones and tissues is distorted resulting in underdeveloped cheekbones, jaw, chin and malformed external ear. Patients may struggle with breathing, eating and hearing impairments as well as with social impediments due to their unusual face structure. As of now circa 95% of TCS cases are associated with mutations in one of the following genes: TCOF1, POLR1D, POLR1C and POLR1B, whereas the remaining 5% cases' genetic cause is yet to be unravelled. We have found a single nucleotide polymorphism (SNP) that appears in TCOF1 exon 21 that changes the proline codon CCC to arginine codon CGC. In order to examine the prevalence of this change, we employed the molecular biology techniques of PCR, Sanger sequencing and restriction enzyme analysis.

References:

1. Marszałek-Kruk, B. A., Wójcicki, P., Dowgierd, K., & Śmigiel, R. (2021). Treacher Collins syndrome: genetics, clinical features and management. Genes, 12(9), 1392.
2. Marszałek-Kruk, B. A., & Wójcicki, P. (2021). Identification of three novel TCOF1 mutations in patients with Treacher Collins Syndrome. Human Genome Variation, 8(1), 36.

Acknowledgement of financial support:

Sulfatide (SM4) serves as a regulatory molecule crucial in the transcription of BOLA2 gene

Jarosław Suchański[1], Weronika Woldańska[1], Safoura Reza[1]

[1] *Wrocław University of Environmental and Life Sciences, Wrocław, Poland*

safoura.reza@upwr.edu.pl, jaroslaw.suchanski@upwr.edu.pl, 115223@student.upwr.edu.pl

Sulfatide (SM4), the simplest, and the most intensively studied sulfated GSL synthesized by the enzyme galactosylceramide sulfotransferase – CST. Increased amounts of sulfatides have been found in various types of carcinomas including breast cancer. The biochemical mechanisms producing altered sulfated glycan structures in cancer cells remain unclear, although understanding it seems to be fundamental in reducing breast cancer cell (BCC) mortality.

Our preliminary data strongly suggest that SM4 can shift the balance in BCC from pro-malignant properties (sulfatides act as malignancy-related adhesive molecules) to reduced-malignant properties (sulfatides act as pro-apoptotic molecules). It seems crucial to clarify how membrane-anchored SM4 can regulate the expression of genes involved in cell invasiveness and apoptosis and may have the opposite effect on the nature of tumor malignancy.

To assess, whether the presence of SM4 affects gene expression associated with invasion promotion or apoptosis we applied Illumina NextSeq 500 sequencing and bioinformatic analyses for identification differentially expressed genes (DEGs) in BCCs overexpressing CST compared to controls. Finally, we correlated high expression of CST down-regulated expression of BOLA2 gene, known to be involved in the apoptosis through CIAPIN1 pathway.

It has been demonstrated that the promoter activity of the BOLA2 gene diminishes with the elevation of sulfatide levels on cell surfaces. Moreover, specific proteins from the STAT family have been identified whose activity is attenuated, implying a potential role in modulating BOLA2 promotor activity. Additionally, it has been observed that one of the subunits of integrin ($\beta 1$) is markedly downregulated under conditions of elevated sulfatide levels, which may be associated, with the regulation of STAT transcription factor expression.

References:

Acknowledgement of financial support:

Sustainable mining: effect of bio(surfactants) on microbial arsenic removal

Agnieszka Pawowska[1]

[1] *Wrocław University of Science and Technology, Wrocław, Poland*

agnieszka.pawlowska@pwr.edu.pl

Sustainable mining aims to reduce the negative effects of mining activities while ensuring that resources are available to future generations. A key aspect is the application of green technologies, such as bioleaching, which helps reduce the environmental impact of the mining industry.

The adsorption of surface-active compounds of both chemical and biological origin alters the surface properties of solid particles. Such phenomena can be used to enhance the extraction of valuable metals from the ore or control the release of metal and metalloids from the solid phase, preventing undesirable effects of bacterial activity in post-mining areas. This study aimed to investigate the physicochemical aspects of bacteria–mineral interactions that occur during the bioleaching of arsenic-bearing waste in the presence of surface-active compounds. The adsorption of biosurfactants and lipopolysaccharides on the mineral surface was demonstrated to alter its charge, influencing the process. The effect of bio-compounds was compared with chemical surfactants such as cetyltrimethylammonium bromide (CTAB) and sodium dodecyl sulfate (SDS). The highest bioextraction efficiency was observed in the presence of rhamnolipids, whereas the lowest efficiency was with adsorbed SDS. Electrokinetic studies revealed that under acidic conditions (pH 2.0 - 2.5), a strongly negative charge of solid particles with adsorbed rhamnolipid increases bacterial adhesion, leading to greater arsenic extraction. On the contrary, SDS adsorbed on a solid surface inhibits bioleaching, which can be used to prevent uncontrolled arsenic release into the environment.

References:

Acknowledgement of financial support: The funding from the National Science Centre (Poland), grant No. 2021/43/D/ST10/02784 is gratefully acknowledged.

Fishes in the net: The role of river network characteristics on fish diversity

Ana Berenice García-Andrade[1], Eduardo Colombo[1], Ismail Ismail[1], Justin Calabrese[1]

[1] *Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Center for Advanced Systems Understanding (CASUS), Görlitz, Germany*

j.calabrese@hzdr.de, e.colombo@hzdr.de, i.ismail@hzdr.de, a.garcia-andrade@hzdr.de

Freshwater fishes are among the most restricted species worldwide because they are fully contained within fragmented networks of water bodies surrounded by land. Given that the natural fragmentation and isolation of these networks have been identified as a generator of the greatest diversity in this group, we need a deeper understanding of their role as drivers of fish diversity. Hints that the evolutionary history and distribution of fishes are closely linked to the geomorphological history of watersheds exist in the literature. For example, some studies have shown that certain watershed traits such as river size, surface area, and natural fragmentation of watersheds are correlated with measures of species diversity. Despite this progress, how the complex interplay between river network structure, watershed characteristics, and species' spatial ecologies drives diversification and biodiversity in freshwater fishes is not yet understood. Here, we combine a global fish occurrence database, a detailed, species-level phylogeny, and a novel dataset on river network structure and watershed traits to comprehensively reveal the determinants of freshwater fish biodiversity at the global scale. The dataset encompasses 11,300+ species distributed across 2,000+ watersheds worldwide, representing approximately 60% of the global diversity of freshwater fishes. To characterize watershed heterogeneity and connectivity we first calculated novel metrics of river network structure including centralization and density, and combined them with geomorphological and climatic characteristics. We then related these variables to fish diversity metrics considering the spatial autocorrelation in the regression analyses. Our preliminary findings indicate that fish diversity is jointly determined by environmental heterogeneity and river network connectivity, highlighting the necessity to account for network structure and characteristics when studying global biodiversity patterns of freshwater species.

References:

Acknowledgement of financial support:

Galactosylceramide-Mediated EGFR Activation in Lipid Rafts: a Mechanism of Drug Resistance in Breast Cancer through AKT Pathway Activation and p53 Down-Regulation

Safoura Reza[1], Jarosław Suchański[1], Michał Grzybek[2], Anita Hryniewicz-Jankowska[3], Aleksander Czogalla[3], Maciej Ugorski[1]

[1] *Wrocław University of Environmental and Life Sciences, Wrocław, Poland*

[2] *Technische Universität Dresden, Dresden, Germany*

[3] *University of Wrocław, Wrocław, Poland*

maciej.ugorski@upwr.edu.pl, safoura.reza@upwr.edu.pl, jaroslaw.suchanski@upwr.edu.pl

The Epidermal Growth Factor Receptor (EGFR) plays a significant role in developing and progressing various cancers, including breast cancer (BC). Its role in promoting cell proliferation, survival, and metastasis makes it an important target for therapeutic interventions. Despite this, EGFR-directed therapies in BC have faced numerous challenges, primarily due to the complex molecular landscape of the disease and the development of resistance mechanisms. It was shown that one of the mechanisms, driving the drug resistance (DR) of BC cells involves galactosylceramide (GalCer) [1], a glycosphingolipid known for its anti-apoptotic properties [2]. GalCer has been implicated in BC cell DR by downregulating the tumor suppressor p53, a process which simultaneously downregulates the expression of pro-apoptotic TNFSF1B and TNFSF9 and upregulates the expression of Bcl-2, affecting at the same time extrinsic and intrinsic (mitochondrial) apoptotic pathways [1].

In the present study, we show that GalCer downregulates the expression of p53 by inducing the ligand-independent phosphorylation of EGFR in lipid rafts, which causes the activation of the AKT signaling pathway, the central player in cell survival and proliferation, and AKT-dependent increased expression of E3 ubiquitin-protein ligase MDM2. The GalCer-dependent activation of EGFR represents a new mechanism by which glycosphingolipids, regulate EGFR-mediated signaling pathways.

References:

1. Suchanski J, Reza S, Urbaniak A, Woldanska W, Kocbach B, Ugorski M. Galactosylceramide Upregulates the Expression of the BCL2 Gene and Downregulates the Expression of TNFRSF1B and TNFRSF9 Genes, Acting as an Anti-Apoptotic Molecule in Breast Cancer Cells. Cancers (Basel). 2024 Jan 17;16(2):389.

2. Owczarek TB, Suchanski J, Pula B, Kmiecik AM, Chadalski M, Jethon A, Dziegiel P, Ugorski M. Galactosylceramide affects tumorigenic and metastatic properties of breast cancer cells as an anti-apoptotic molecule. PLoS One. 2013 Dec 31;8(12):e84191.

Acknowledgement of financial support: National Science Center, Poland (Grant no. 2019/35/B/NZ5/-01392).

Chemical robotics for outreach and autonomous laboratories

Johannes Guenzl[1], Miroslav Položij[2], Thomas Heine[1,2]

[1] *Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Center for Advanced Systems Understanding (CASUS), Görlitz, Germany*

[2] *Technische Universität Dresden, Dresden, Germany*

johannes.guenzl@hzdr.de, miroslav.polozij@tu-dresden.de, thomas.heine@tu-dresden.de

Chemistry is not only the science of constructing new molecules and materials, but also the craft of performing syntheses. The latter aspect has changed very little over the last century despite tremendous progress in robotics, automation and digitalization in other scientific domains. To overcome the challenges of the 21st century, chemistry needs to become more reproducible, time-efficient and reduce its ecological impact. Autonomous robotic chemistry systems help achieve these goals and will reshape the public perception of chemistry as a modern, precise science.

To promote our emerging autonomous chemistry platform, the Heine group at the Dresden University of Technology uses two illustrative chemical robots in our outreach activities. These are constructed from LEGO® bricks and were designed by Gerber et al. [1]. One of them can perform simple pipetting tasks such as color mixing or dilution series, allowing students to program it themselves. The second robot illustrates the automation of chemical synthesis through automatic preparation of simple cocktails. Both robots have proven effective in promoting chemistry at events such as the long night of science and Girls' day.

Aside from their success in popularizing science, these robots illustrate the potential of real robotic chemistry platforms. The system in development at the Heine group aims for the precise control of liquid-phase syntheses. This is achieved by applying several in-situ spectroscopies simultaneously and evaluating the data using machine learning models. Predictions and results are enhanced using theoretical chemistry calculations.

References:

1. Gerber LC, Calasanz-Kaiser A, Hyman L, Voitiuk K, Patil U, Riedel-Kruse IH (2017) Liquid-handling Lego robots and experiments for STEM education and research. PLoS Biol 15(3): e2001413. https://doi.org/10.1371/journal.pbio.2001413

Acknowledgement of financial support:

Production relocation in the global economy - new trends

Katarzyna Witczyńska[1]

[1] *University of Wrocław, Wrocław, Poland*

katarzyna.witczynska@uwr.edu.pl

Current trends in the global economy show an increasing tendency to relocate production abroad. Companies are faced with the challenge of coping with rising energy prices, inflation and interest rates, which is causing them to think about relocating their production sites1. A survey by the Federation of German Industries found that 16% of the companies surveyed are already actively relocating parts of their production abroad, while another 30% are considering doing so.

In practice, however, it turns out that relocating production back to Europe is fraught with challenges, as many current employees were not even born when the company's division was outsourced. The reasons for so-called reshoring are diverse and range from political tensions to trade conflicts, especially between the US and China.

These developments are of crucial importance for CFOs and company managers who must adapt their production strategies to remain competitive while minimizing the risks associated with global production relocation.

References:

1. Bhagwati, J. [2004]. In defence of globalization. Oxford University Press, Oxford.
2. Coyle D. [2020], Markets, State, and People: Economics for Public Policy, Princeton University Press, Princeton.
3. Porter M.E. (1996), What Is Strategy, "Harvard Business Review", No. 1112.
4. Poynter T.A., White R.E. (1984), The Strategies of Foreign Subsidiaries: Responses to Organisational Slack, "International Studies of Management and Organizations", Winter.
5. Porter M. [2011], Competitive Advantage of Nations: Creating and Sustaining Superior Performance, Simon and Schuster, New York.

Acknowledgement of financial support: Thank you for the cooperation the Economic Institute in the Wroclaw University.

How to (numerically) calculate tortuosity in porous media?

Maciej Matyka,[1] Damian Śnieżek,[1] Sahrish Naqvi,[1] Dawid Strzelczyk,[1] Krzysztof Graczyk[1]

[1] *University of Wrocław, Wrocław, Poland*

maciej.matyka@uwr.edu.pl

Tortuosity is the third parameter (after porosity and permeability) most often computed in the investigation of transport through porous media. It characterizes the elongation of emergent diffusive, hydrodynamic, or electric transport paths.

In this poster, we will present several ways of tortuosity computation. Initially, we spotlight the streamline-based approach. To facilitate this, our docker-integrated OpenFOAM (FVM) framework —engineered to construct porous media and execute pore-scale fluid flow simulations efficiently — will be supplemented with Python script to compute multiple streamlines. We will then compare results derived from this method with those from the velocity-based procedure. The poster will shed light on the challenges posed by these methodologies, especially in conditions like the inertial regime where non-linear dynamics become prominent. Additionally, the discourse will touch upon meshless interpolation techniques suitable for streamlines and the Lattice Boltzmann solver in tortuosity. In conclusion, we will explore a novel procedure utilizing a deep learning Convolutional Neural Network (CNN) approach designed to determine tortuosity in randomized porous media. This approach proficiently calculates hydrodynamic and diffusive tortuosity.

References:

Acknowledgement of financial support: This work was supported by NCN OPUS LAP grant no. 2021/43/I/ST3/00228.

Bayesian analysis of the dense matter equation of state.

A. Ayriyan,[1] D. Blaschke,[1] O. Ivanytskyi,[1] L. Turko,[1] E. Zherebtsova[1]

[1] *University of Wrocław, Wrocław, Poland*

alexander.ayriyan@uwr.edu.pl

Bayesian inference is a powerful framework for probing the characteristics of equations of state (EoS) of nuclear matter under extreme conditions. In determining the intricate relationship between pressure and density, two distinct Bayesian methodologies emerge: the 'agnostic' and the 'educated' approaches. The agnostic strategy treats the equation of state only as a relation between pressure and density, making minimal assumptions about underlying physics. It relies solely on observational or experimental data to inform the probabilistic distribution of possible equations of state. The 'educated' strategy analyzes the physical parameters defining the equation of state, incorporating prior knowledge from physical laws or empirical observations to constrain possible equations of state. The poster outlines the methodology, benefits, and insights gained from employing an 'educated' Bayesian inference in the study of equations of state of dense nuclear matter.

References:

1. D. Blaschke, A. Ayriyan, M. Cierniak, A. G. Grunfeld, O. Ivanytskyi, M. Shahrbaf. Special point "trains" in the M-R diagram of hybrid stars. EPJ Web of Conferences 274, 07011 (2022). DOI:10.1051/epjconf/202227407011.

2. M. Shahrbaf, S. Antić, A. Ayriyan, D. Blaschke, A. G. Grunfeld. Constraining free parameters of a color superconducting nonlocal Nambu–Jona-Lasinio model using Bayesian analysis of neutron stars mass and radius measurements. Phys. Rev. D 107, 054011 (2023). DOI:10.1103/PhysRevD.107.05-4011.

3. D. Alvarez-Castillo, A. Ayriyan, G.G. Barnaföldi, H. Grigorian, P. Pósfay. Studying the parameters of the extended σ-ω model for neutron star matter. Eur. Phys. J. Spec. Top. 229, 3615–3628 (2020). DOI:10.1140/epjst/e2020-000106-4.

4. D. Alvarez-Castillo, A. Ayriyan, S. Benic, D. Blaschke, H. Grigorian, S. Typel. New class of hybrid EoS and Bayesian M - R data analysis. Eur. Phys. J. A 52, 69 (2016). DOI:10.1140/epja/i2016-16069-2.

Acknowledgement of financial support: The work was supported by NCN under grant No. 2021/43/P/-ST2/03319.