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MEMBRANE TECHNOLOGY FOR WASTEWATER TREATMENT, REUSE, AND VALUABLE CHEMICAL RECOVERY FROM GEOTHERMAL WATER

Samuel Bunani

University of Burundi

My research interest is mainly in wastewater treatment processes for water reuse/reclamation and the recovery of valuable elements from various water resources. I am very interested in environmental issues, especially the management of municipal and industrial wastewater effluents. In this perspective, using my expertise and experience in water sanitation processes, my main goal is to develop efficient technologies and strategies for a safe water supply and a clean environment by managing the available water resources and wastewaters at lab and mini-pilot scale for industrial-scale implementation. in this context, I am mostly interested in water quality analysis, membrane separation technology (NF and RO) for water reuse, electromembrane processes for wastewater management using electrodialysis (ED), and the recovery of valuable elements from water resources using bipolar membrane electrodialysis (BMED). My interest includes inorganic water traces' decontamination by using ED and ultrapure water production by using electrodeionization (EDI) processes.

FUNCTIONING OF MARINE ECOSYSTEMS—A BENTHIC PERSPECTIVE

Monika Kędra

Institute of Oceanology,

Polish Academy of Sciences

Dr. Monika Kędra is an Associate Professor at the Institute of Oceanology, Polish Academy of Sciences (IOPAN) in Sopot, Poland. Dr. Kędra was the vice-chair of the Polish Young Academy (2017–2019) and is currently a member of the Global Young Academy Executive Committee. She holds an M.S. degree in Oceanography and a Ph.D. in Earth Sciences—Oceanology. Her research includes climate change impacts on marine ecosystems functioning, and in particular, benthic carbon and nutrients cycling, pelagic-benthic coupling, and marine food webs. Most of her work is conducted in the Arctic Ocean and the Baltic Sea.

During this presentation, she will talk about the benthic (sea floor) communities and their role in the marine ecosystem functioning in temperate (Baltic Sea) and polar (Arctic Ocean) seas. The role of environmental conditions and the quality and quantity of organic matter—the main food source—in shaping the benthic community in the Arctic regions will be discussed. Next, the impact of benthic organisms and their activities on the carbon and nutrient fluxes in the coastal zones of the southern Baltic Sea will be presented. Finally, the presentation will conclude with the expected shifts resulting from ongoing climate change.

INTRODUCTION TO NEGATIVE CARBON FOOTPRINT ALIVE STRUCTURAL PRODUCTS

Ajitanshu Vedrtnam

Mineral and Energy Economy Research Institute, Polish Academy of Sciences, Poland

Department of Mechanical Engineering, Invertis University, Bareilly, UP, India-243001

Magdalena Wdowin

Mineral and Energy Economy Research Institute, Polish Academy of Sciences, Poland

The globe is concerned about the rising level of CO_2, as it contributes to climate changes, snow cover melting, and the greenhouse effect. The present work involves the development of construction products that absorb CO_2, similar to trees, for strengthening and trapping it repeatedly, resulting in an overall negative carbon footprint. These products consist of bacterial concrete, a vascular system, and a CO_2 selective filter. The synthesis and testing of Zeolitic Imidazolate Framework-8 (ZIF-8) based novel filters for CO_2 capture are reported. The ZIF-8 nanopowder was synthesized, and the cellulose fibers were prepared using the kraft pulping process. Varying the Zn^{2+} molar ratios in the synthesis solution resulted in different particle sizes of ZIF-8 nanopowder. Furthermore, the cellulose-based ZIF-8 Air Filters (ZCAFs) with cellulose powder are prepared. The morphologies of the nanopowders and filter material are examined, and capacity for capturing CO_2 is evaluated. Initial experimental results for bacterial concrete and the vascular system are found to be encouraging. This work should contribute to the production of sustainable construction products.

PHYTOREMEDIATION OF CONTAMINATED ENVIRONMENTS USING HALOPHYTES: TARGETING CIRCULAR ECONOMY

Tallou Anas
Alessandro Gaetano Vivaldi
Francesco Abbatantuono
Salem Alhajj Ali
Department of Soil, Plant and Food Sciences, University of Bari "Aldo Moro", Italy

Francisco Pedrero Salcedo
Centre of Applied Biology and Soil Sciences (CEBAS), *Spain*

Due to anthropogenic activities, potentially toxic elements (PTEs) have disrupted our ecosystems' natural balance. These dangerous substances can infiltrate the food chain, affecting environmental balance and human life. To preserve our natural environment for future generations, scientists must look for eco-friendly alternatives. Each year, about 300 million tons of PTEs from industrial and consumer items, including Cr, Cu, Zn, As, Cd, Pb, and Sn, make their way into natural water sources. Halophyte plants are found worldwide and grow in various places, including coastal zones, dunes, high-salinity environments, and inland deserts. They may also withstand PTEs stress due to evolved morphological and physiological characteristics, such as reduced heavy metal intake through the root system. PTE contamination causes agriculture yield losses, increases environmental concerns about human well-being, and causes a significant drop in marine and coastal ecosystem biodiversity. Halophytes are plants that can flourish in extreme conditions, such as high salinity and heavy metal toxicity. This work emphasizes the role of halophyte plants in terms of PTEs phytoremediation as a long-term strategy for polluted environmental ecosystem restoration, which is in line with the current European Green Deal strategy for a neutral Europe climate by 2050.

Keywords: Phytoremediation; Halophytes; Contaminants; Toxic elements; Blue economy.

WATER IN CIRCULAR ECONOMY

Marzena Smol

Mineral and Energy Economy Research Institute,

Polish Academy of Sciences, Poland

This paper presents the importance of the water sector in the circular economy (CE) model. in the water sector, the main attention is paid to improving the rational management of primary resources such as water, energy, and biogenic raw materials (nitrogen, phosphorus), and the sustainable management of secondary resources (waste) such as sewage, sewage sludge, or sewage sludge ash. Water companies that align with the CE model focus on a new perspective on the municipal wastewater stream as a source of water, energy, and secondary raw materials while maintaining the basic requirements of the wastewater treatment plant (WWTP), such as ensuring sanitary safety and optimizing the operating costs of the treatment plant.

On the European level, water reuse from municipal wastewater is becoming more and more important due to the new regulations in this field (EU 2020/741). Water reuse is defined as the treatment of already used water to a quality that allows it to be reused in various utility processes. Water reuse can be applied in various sectors, such as the industrial sector, agricultural sector, services sector, as well as individual households. Such solutions may bring economic benefits (no need to draw water from the network) and environmental benefits (no need to draw water from the intake and protection of water resources).

Acknowledgments: This paper is prepared based on results obtained under the Subvention of the Division of Biogenic Raw Materials in the Mineral and Energy Economy Research Institute, Polish Academy of Sciences, and the project 'Water-CE-management in practice—developing comprehensive solutions for water recovery and raising awareness of the key role of water in the transformation process towards a circular economy (CE)', co-financed (EUR 280,000) by Iceland, Liechtenstein, and Norway through the EEA and Norway Grants.

MONITORING LEAD CONCENTRATION IN THE SURROUNDING ENVIRONMENTAL COMPONENTS OF A LEAD BATTERY COMPANY: PLANTS, AIR, AND EFFLUENTS—CASE STUDY, KENYA

Jeremiah Otieno

Gdansk University of Technology

Lead (Pb) pollution from smelters and lead–acid batteries has become a serious problem worldwide owing to its toxic nature as a heavy metal. Stricter regulations and monitoring strategies have been formulated, legislated, and implemented in various parts of the world on heavy metal usage. Developed countries such as the USA and in Europe largely operate within the set standards; however, developing countries such as Kenya, Nigeria, and India, with limited regulatory capacity, resources, and sufficient data, face poor Pb waste management and exposure of the population to health risks.

This study assessed the pollution concerns from Associated Battery Manufacturers (East Africa) Limited (ABM), located in the Nairobi Industrial Area in Kenya. Samples of air, extracts from plants (leaves), and factory wastewaters were taken from different operational units, prepared, and analyzed with Atomic Absorption Spectrometry (AAS). Pb traces remained fairly controlled with averages of 1.24 ± 0.42 parts per million (ppm), 1.21 ± 0.02 ppm, and 0.29 ± 0.01 ppm in the air, plant extracts, and effluents, respectively.

The conducted research shows that the obtained lead concentrations in the air, wastewater, and surrounding plants exceeded the recommended standards and are potentially harmful not only to workers but also to the surrounding villages.

WASTE TO WEALTH: BIOENERGY PRODUCTION FROM SEWAGE SLUDGE RECOVERY

Lamiaa Chab

University of Tuscia

The presentation focuses on the concept of "Waste to Wealth: Bioenergy Production from Sewage Sludge Recovery." It explores the potential of sewage sludge as a resource and its conversion into bioenergy through anaerobic digestion. The presentation highlights this approach's environmental, energy, and economic benefits, including reduced greenhouse gas emissions, a sustainable source of renewable energy, and job creation. However, it also addresses the challenges associated with technical aspects, regulations, and public perception. By promoting collaboration and innovative solutions, we can unlock the valuable potential of sewage sludge for bioenergy production and contribute to a more sustainable future.

Keywords: Bioenergy production; sewage sludge; resource recovery.

BREAKING THE COLOR BARRIER: MYCOREMEDIATION AS AN ENVIRONMENTALLY FRIENDLY TECHNOLOGY FOR EXPELLING SYNTHETIC DYE FROM TEXTILE WASTEWATER

Ruchi Upadhyay

Department of Air Protection,

Faculty of Energy and Environmental Engineering,

Silesian University of Technology, Poland

The growth of diverse industries, such as textiles, leather, paper, and food, can provide any nation with a solid economic foundation. However, industrialization and modernization have resulted in environmental degradation, as these industries are responsible for the production of vast quantities of water contaminated with toxic chemicals, such as various types of synthetic dyes, due to inadequate waste management.

Mycoremediation has emerged as a green technology to combat intractable compound pollution in a cost-effective and efficient manner and contribute to sustainable development. The White Rot Fungi—Trametes versicolor (CB8) strain was chosen for dye removal using the biosorption mechanism. Two triphenylmethane dyes—Brilliant Green (BG) and Crystal Violet (CV) were taken at two different concentrations (200 and 400 mg/L) at their natural pH. It showed enhanced dye removal efficiency when fungal biomass was immobilized on the solid synthetic support-sponge. At a higher BG concentration, the free fungal biomass was showing desorption of the dye, whereas immobilized fungi showed approximately 80% removal in just 6 hours.

The chosen fungal strain was less efficient for CV dye removal compared to BG, as it removed approximately 40% of CV dye after 6 hours at a 200 mg/L concentration. The experimental results were promising for dye removal using the biosorption mechanism, and it required optimization of the process so that it will be able to treat real textile wastewater within no time. It will pave the way for the development of a large-scale optimized bioreactor capable of treating effluent containing dye.

Keywords: mycoremediation; synthetic dyes; sorption; Trametes versicolor (CB8); triphenylmethane dye.

SIZE-EFFECT OF CoO-BASED THIN-FILM CATALYSTS IN CO_2 METHANATION REACTION

Niloofar Mohammadpour
Hanna Kierzkowska-Pawlak
Jacek Balcerzak
Jacek Tyczkowski
Department of Molecular Engineering,
Faculty of Process and Environmental Engineering,
Lodz University of Technology, Poland

Paweł Uznański
Centre of Molecular and Macromolecular Studies,
Polish Academy of Sciences, Poland

The use of thin-film catalysts in the new generation of structured reactors is gaining increasing attention due to their potential applications in various demanding processes such as CO_2 valorization. in the current research, the performance of CoO-based catalysts with size-controlled nanostructure in the CO_2 methanation reaction was investigated. The catalysts, in the form of thin films, were prepared using the plasma-enhanced chemical vapor deposition (PECVD) technique on Kanthal steel meshes. Varied precursor ($CpCo(CO)_2$) flow rates were applied, while deposition power and carrier gas flow rates were kept constant. The as-deposited thin films, in the form of amorphous CoOX, were thermally treated in argon at 400°C. The surface composition of samples was investigated by X-ray photoelectron spectroscopy (XPS), while the structure of the thin film was analyzed by X-ray diffraction (XRD).
The analysis of the surface composition demonstrated that, irrespective of precursor flow rate, the surface chemical composition of samples was the same under the applied plasma parameters. It was found that the nanostructure of the catalyst is in the form of face-centered-cubic (fcc) CoO dispersed in the carbon matrix with a graphite-like structure. The CoO sizes of nanocrystallites increased from 2 nm to 11 nm with the increasing precursor flow rate.
The catalysts were tested in a CSTR reactor at a temperature range of 200–400°C with a gas flow of reactants (H_2/CO_2 = 4). A general tendency to de-

crease CO_2 conversion, while increasing the CoO nanocrystallite size, was observed while maintaining the same CoO density. The results indicate that CO_2 methanation is a structure-sensitive reaction over plasma-prepared CoO-based catalysts. We have also shown that the cold plasma deposition technique allows for the fabrication of nanostructured thin-film catalysts in a controllable way and may offer significant potential for improving the performance of CO_2 conversion.

SPATIAL VARIATION ANALYSIS OF CHLOROPHYLL CONCENTRATION USING SENTINEL-3 OLCI IMAGERY IN THE BAY OF BENGAL ALONG THE SHORES OF THE CHENNAI DISTRICT, INDIA

Kaushik Karishma

Warsaw University of Technology

At present, marine pollution, resulting from anthropogenic activities and global climate change, is one of the most concerning environmental issues related to the degradation of the marine ecosystem. It not only affects the marine ecosystem but also impacts human beings. Several parameters can be measured using satellites to provide an in-depth observation of marine pollution and changes occurring in oceans, seas, and rivers over time. The author has chosen chlorophyll detection of a specific marine area in the Bay of Bengal sea in the current study.

The Bay of Bengal covers around 2.172 million square kilometers of area across India, Bangladesh, and Myanmar, with significant river deltas like the Ganga and Brahmaputra rivers. The present study aimed to determine the distribution pattern of chlorophyll concentrations as a factor of phytoplankton abundance in the selected area of Chennai District and its spatial variability. Additionally, the study aimed to evaluate the potential of Sentinel-3 Ocean and Land Color Instrument (OLCI) satellite data for monitoring algal blooms. It's a satellite from the ESA Copernicus group.

Chlorophyll-a (Chlorophyll) related products were tested and monitored for the entire year 2018 using the plug-in with SNAP tool, which assessed their ability to estimate chlorophyll concentration. The results showed that the concentration of chlorophyll was able to relate to the phytoplankton blooms in the study area. The areas with massive phytoplankton blooms showed high chlorophyll values (mg/m^3). The radiance spectrum with a MERIS heritage wavelength shows quite high reflectance values. Simultaneously, bands 11, 8, 6, 4 provided the best results.

Also, the analysis of chlorophyll made on the basis of Sentinel-3A OLCI satellite images could be used for detection, tracking, and delineating phytoplankton blooms in a given area. The techniques used in this study will be

useful in enhancing the ability to track chlorophyll concentration in marine coastal areas and will also help local coastal aquaculture operators and fishing purposes to receive timely and accurate information that can be scientifically and commercially of great importance. This study demonstrated that the new satellite sensors, OLCI, can play a significant role in monitoring chlorophyll concentration in a large area.

Keywords: Chlorophyll; Phytoplankton; OLCI; Sentinel-3; Marine pollution; Spatial distribution; SNAP.

CIVIL, MECHANICAL & MATERIALS ENGINEERING

ON THE DEVELOPMENT OF AUXETIC CEMENTITIOUS MATERIALS FOR ENERGY PRODUCTION

Jennifer Udebunu

Department of Materials Engineering and Construction Processes,
Faculty of Civil Engineering,
Wroclaw University of Science and Technology, Poland

The development of auxetic cementitious materials for energy production has emerged as a promising avenue for sustainable and efficient energy conversion. Auxetic materials, characterized by their negative Poisson's ratio, exhibit unique mechanical properties that can be harnessed to enhance energy harvesting and storage capabilities. This abstract provides an overview of the research and development efforts in the field of auxetic cementitious materials for energy production.

The development of auxetic cementitious materials involves incorporating auxetic fibers or particles into the cementitious matrix, thereby imparting the desired auxetic behavior. This innovation opens up new possibilities for energy production, with potential applications ranging from pavements to buildings and infrastructure. By leveraging the auxetic behavior of these materials, energy conversion efficiency can be significantly improved, leading to enhanced energy harvesting from various sources.

The synthesis and characterization of auxetic cementitious materials have been the focus of extensive research. Different approaches, including the use of various types and concentrations of auxetic fibers or particles, have been explored to optimize the auxetic behavior and overall performance of the materials. Mechanical, thermal, and energy conversion properties are evaluated to ensure their suitability for energy production applications.

In terms of applications, auxetic cementitious materials offer significant advantages. They can be integrated into pavements to harness energy from vehicular movement, thereby providing a sustainable energy source. In the construction industry, the incorporation of these materials in buildings promotes energy-efficient structures. Additionally, auxetic cementitious materials can be utilized in infrastructure such as bridges and tunnels, enabling sustainable energy solutions in these critical components.

While the development of auxetic cementitious materials for energy production shows promise, there are still research gaps that need to be addressed. Standardized testing methods for evaluating material properties and long-term durability assessments are necessary to ensure reliability and performance over time. Furthermore, the optimization of material behavior and the exploration of novel materials and composites are crucial to unlock the full potential of auxetic cementitious materials for energy production.

In conclusion, the development of auxetic cementitious materials for energy production presents a novel approach to address the increasing demand for sustainable energy solutions. These materials offer unique properties that can enhance energy conversion efficiency, making them suitable for applications in pavements, buildings, and infrastructure. However, further research is needed to address the existing research gaps and optimize the material's behavior. With continued advancements, auxetic cementitious materials have the potential to contribute significantly to sustainable energy production and storage, paving the way for a greener and more efficient future.

SUSTAINABLE SOLUTIONS FOR HIGH-QUALITY PAVEMENT CONCRETE: EXPLORING THE IMPACT OF RECYCLED COARSE AGGREGATES AND WASTE FOUNDRY SAND ON SLAG-BASED ALKALI-ACTIVATED MIXES

Akhila Sheshadri, Shriram Marathe

Department of Civil Engineering, NMAM Institute of Technology, India

Alkali Activated Concrete (AAC) is an environmental friendly and sustainable alternative for the carbon footprint problems associated with the conventional Ordinary Portland Cement (OPC) based cementitious mixes for the infrastructural development. Since, the aggregates comprise the majority of the concrete volume; it is also a challenge in front of future structural engineers to minimize the usage of natural aggregates in concretes, thereby reducing the exploitation of natural resources and enhance the reuse of industrial waste materials. This paper presents the results of research on eco-friendly slag-based AAC which incorporates the Waste Foundry Sand (WFS), obtained from foundry industry and Recycled Coarse Aggregate (RCA), obtained from local construction and demolition waste into concrete system. The mix proportion was designed for strength of 50 MPa by following the recent Indian standard guidelines for high quality paver applications, and through the literature support, the further modifications in mix proportion is carried out to obtain the proportioning for slag based-AAC mixes. Based on the compressive strength results, the optimized WFS and RCA content were obtained to be 20% and 50% (by volume), respectively their conventional counterparts in the production of AAC mixes. Further, the mechanical properties such as unit weight, water absorption, split-tensile strength, and flexural strengths were evaluated and analyzed. With the utilization of 20% WFS with 50% RCA in AAC mixes, the disposal problems associated with WFS and RCA could be addressed to a great extent, which in-turn contributes to the sustainable infrastructural development goals of the present day mankind.

APPLICATION OF LOW-COST WEB-BASED WIRELESS STRUCTURAL HEALTH MONITORING RASP SYSTEMS FOR BRIDGE STRUCTURES

Duc Cong Nguyen[1], Marek Salamak[1], Andrzej Katunin[2]

[1] *Department of Mechanics and Bridges, Faculty of Civil Engineering, Silesian University of Technology, Poland*

[2] *Department of Fundamentals of Machinery Design, Faculty of Mechanical Engineering, Silesian University of Technology, Poland*

Structural Health Monitoring (SHM) technologies have been widely popular applied in numerous interdisciplinary research areas devoted to the monitoring and evaluation of structural health state and life cycle assessment for civil structures and infrastructures under natural hazards and climate change with potential industrial applications, as well as latest advances and innovations in both the management of real-time emergency situations and maintenance needs in recent trends, especially in the high-tech strategies of Virtual Bridge Information Modelling (VBrIM), Internet of Things (IoTs), Web of Things (WoTs), Industry 4.0. This study presents vibration-based SHM using the Raspberry Pi (RASP) system and low-cost micromachined microelectromechanical systems (MEMS) accelerometers. The low-cost innovative SHM system includes acquisition hardware MEMs of wireless sensor networks (WSN) to record the dynamic responses of the structure and transfer historical data sets through the mobile 3G/4G SIM card, smart Wi-Fi and the web-based platform. Sensor data sets are managed to upload to the Web-based Server for interactive display of real-time data information and event-structural historical behaviours in the Web mapping service (WMS), in which the positions of sensors and structures are integrated into the virtual digital twin (DT) lab with all-in-one solution to interface with viewers to monitor the health state of the structure. The automatic alert system sets the minimum and maximum threshold values of vibration signals to implement in SHM systems that could send short message service (SMS) notifications through Telegrams online.

APPLICATION AND LIMITATION OF SELF-HEATING EFFECT IN POLYMER-MATRIX COMPOSITES UNDER FATIGUE LOADING

Jafar Amraei
Andrzej Katunin
Department of Fundamentals of Machinery Design,
Faculty of Mechanical Engineering, Silesian University of Technology, Poland

The superior dynamic performance of polymer-matrix composite (PMC) structures has motivated industries such as wind turbine, civil, and aerospace to implement PMCs for different purposes. When PMCs are cyclically loaded, the heat is stored due to their low thermal conductivity and viscoelastic nature, leading to the temperature growth on the specimen surface, called self-heating temperature. Its intensity depends on material properties and fatigue loading parameters. If this temperature is significantly lower than its critical value, the heat stored can advantageously be used as an alternative heat source in a nondestructive damage identification technique for PMC structures, called self-heating-based vibrothermography (SHVT) developed by this research group. Nevertheless, if self-heating temperature is close to or higher than its critical value, the fatigue performance of PMC will negatively be dominated by this phenomenon. This accelerates damage accumulation, leading to intensive structural degradation and eventually premature thermal fatigue failure. For a PMC specimen with arbitrary material properties, this can happen under high loading frequency and/or stress/strain level. To limit the occurrence of such a catastrophic situation, the fatigue experiments can be performed at low frequency (i.e. 5 Hz), which would disadvantageously be time-consuming, requiring roughly 6 years (almost one third of life span of a wind turbine blade) for conducting one experiment in very-high-cycle-fatigue range up to 109 cycles. The viable solution is to safely accelerate the fatigue experiments under higher frequency but prevent the self-heating effect by cooling down the specimen surface using an efficient cooling technique, which we are currently working on.

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SMART BRIDGE INSPECTION METHODS USING BIM TECHNOLOGY

Muhammad Fawad[1]
Marek Salamak[1]
Shahab Shahid[2]

[1] *Department of Mechanics and Bridges, Faculty of Civil Engineering, Silesian University of Technology, Poland*

[2] *Department of Power Electronics, Electrical Drives, and Robotics, Faculty of Electrical Engineering, Silesian University of Technology, Poland*

This study has analyzed the existing SHM system of a bridge for its automation using BIMification approach. This analysis started with load testing followed by the FEA of the bridge. It has been done to compare the numerical calculations with the experimental ones. To simplify the FE model generation, a novel methodology is developed which can generate a BIM-based FE model using the Visual Programming Language scripts in Dynamo. This script can be exported to any FE software to develop the FE model. Further, BIMification is developed by integrating BIM model of the bridge with its SHM system. For this purpose, smart sensors are deployed to BIM model of the bridge. Consequently, the BIM model is used to manage and monitor the SHM system and to control its sensors. These sensors are then linked with the self-generated IoT platform (coded in Arduino); developing a smart SHM system of the bridge.

CONCRETE-BASED WATER FILTER FOR LOW-COST TREATMENT OF INDUSTRIAL WASTEWATER

Murugan Muthu

Department of Materials Engineering and Construction Processes, Wrocław University of Science and Technology, Poland

We developed a permeable concrete mix based on geopolymer binder and then examined its potential against removal of toxic heavy metals from simulated industrial wastewater. This porous concrete was prepared with a minimum allowable porosity range, making it strong, less permeable, and highly efficient in the removal of metal pollutants, compared to normal permeable concrete. The use of geopolymer binder improved the resistance of the concrete to acids. The cost estimate showed that using this permeable concrete in place of practical treatment units could be cost-saving up to 66 times. In general, the study proposes low-carbon permeable concrete as an affordable and practical system for the removal of toxic heavy metals from industrial wastewater (electroplating and manufacturing automobile battery manufacturing).

EFFICIENT UTILIZATION/REUSE OF BUILDING MATERIALS RESULTING FROM MASSIVE DESTRUCTION IN WAR RAVAGED REGION—A CASE STUDY OF UKRAINE AND SOME SELECTED AFRICAN COUNTRIES

Emmanuel Oluwasegun

Faculty of Civil Engineering,

Wrocław University of Science and Technology, Poland

Conflicts and wars have damaged and wrecked critical infrastructure, including houses, hospitals, schools, roads and gas supply systems. Several wastes generated from the destroyed infrastructure affect the safety, health and environment. Restoration and reconstruction present the re-establishment of lost properties or provision of better and more robust housing that existed before the conflicts. The waste management resulting from the destruction during the conflicts needs to be checked. Construction and demolition (C&D) waste materials are produced when a new building or civil engineering products are constructed and when old buildings and civil structures are refurbished or demolished, destroyed including demobilization activities. This work aim to examine the efficient utilization and reuse of building materials arising from the massive destruction during the period of wars. The objectives would be to assess the extent of reuse of the C&D materials resulting from the destroyed structures in the selected countries. Secondly, compare the life cycle assessment of destroyed buildings from the end-of life approach, categorization of the various wastes resulting from the destruction using a multi-factorial approach. The determination of the utilization rate of the materials generated from the destruction site using system dynamic modelling (SDM). The research objectives will be achieved by providing a comprehensive review of literature, case studies, interviews of stakeholders in the selected countries and using the SDM to develop a model to predict the utilization rate. This research will be valuable to industry practitioners, governments of nations impacted by armed conflicts, and international organizations providing aid for the restoration and rebuilding of the affected countries.

STUDY IN THE USE OF POLARIZATION MAINTAINING FBG SENSORS FOR GUIDED WAVE MODE SEPARATION

Sara Sarbaz

Institute of Fluid Flow Machinery,

Polish Academy of Sciences, Poland

Guided wave technology is commonly employed for detecting damage in thin-walled structures owing to its capability to propagate over long distances. However, the presence of multiple modes, mode conversion, and reflections from boundaries and discontinuities in complex structures presents a challenge in signal processing. In this study, using polarization-maintaining fiber Bragg grating (PM-FBG) sensors for guided wave mode separation is proposed to tackle this challenge. PM-FBG sensors can detect the polarization state of guided waves and differentiate between different modes based on their polarization characteristics. We present experimental results that investigate the effectiveness of PM-FBG sensors for guided wave mode separation. The study involves analyzing the impact of various propagation angles on a plate instrumented with PM-FBG sensors. The proposed approach provides a simple solution for guided wave mode separation, which could have implications for reference free health monitoring techniques.

FBG SENSORS BASED GUIDED WAVE ANALYSIS FOR STRUCTURAL HEALTH MONITORING

Sultan Ahamad

Institute of Fluid Flow Machinery,

Polish Academy of Sciences, Poland

Structural health monitoring (SHM) techniques improve structure safety and reliability by detecting damage and providing critical information. Recently, the guided wave-based SHM methodology has been extensively used with Fiber Bragg grating (FBG) sensors. The excitation of waves is very important in guided wave-based methodology, and it is generally performed by the actuation of piezoelectric transducers (PZTs). More research into different actuations by different PZTs and their sensing by FBGs is needed. The proposed method involved signal excitation (actuation) with different-sized PZTs and sensing with pair of FBGs. These FBGs were attached to the aluminum plate's top and bottom surfaces. There was a noticeable difference in the results obtained by actuation of different sizes of PZTs. This study demonstrated the effect of PZT size on the generated guided waves. It will be useful for future research because actuation is an important part of guided wave-based SHM. As well as the sensing on both sides of the plate by FBGs is also useful for suppressing some of the propagating modes.

RECYCLING AND MIMICKING COMPOSITES WITH 3D PRINTING

Mohammad S. Harb

American University of Beirut, Lebanon

Recent studies have demonstrated that carbon fibers could be used to modify the performance of 3D printed parts efficiently. However, a lot of the cost of additive manufacturing (AM) composite materials is in that carbon fiber, which results in a high cost of 3D printed high-performance composite products. To target the cost issue of carbon fiber usage in 3D printing, we investigate the possibility of upcycling carbon fiber waste into additive manufacturing row material. Our work aims to answer the following questions: would it be viable to reuse an already cured carbon fiber composite enriched with thermosetting polymer in additive manufacturing? What are the methods and processes needed to recycle such material and be used in additive manufacturing? And finally, what are the residual properties of the reclaimed batch material compared to its original when used in 3D printed structures? 3D printing continues to provide promising applications in different fields, its integration into critical structures demands a solid knowledge of the integrity of a printed object. Ultrasonic nondestructive testing (NDT) could be used to inspect the integrity of the structure, and characterize its properties. Additionally, investigating ultrasound in AM would improve our understanding of the mechanics of waves and their interaction with defects. Discontinuities could be easily modeled using AM to mimic actual composite damages with less time, higher precision, minimal waste, and thus cheaper cost.

LIFE CYCLE IMPERATIVES IN CONSTRUCTION ENGINEERING

Vsevolod Nikolaiev

Wroclaw University of Science and Technology, Poland

The life cycle concept is the modern basis of engineering and construction management. In last decade, that each function of LC engineering has developed its methodology. Real property management is limited by cash flow management either from the commercial (lease) use of the object, or from its sale. The main focus of real estate management is design and construction of efficient object, long-term preservation of its consumer quality, maintenance planning, based on optimizing cost or value of the LC. Asset management shows how the strategic goal and functions of management determine the appropriateness of the acquisition, maintenance and disposal of assets as financial and accounting objects within the whole building. Instead, the building management considers technical and economic issues depending on the purpose of the project. Facility management, in our opinion, considers efficient use of the space in functioning of building.

Last time, especially in connection with BIM, LC started to orient not only on the whole object but on its structural elements. It means also that BIM helps to design and manage LC of the construction systems composed by the elements.

Finally, let's look on BIM as a tool for LC engineering. Real BIM, unlike 3D design, must support all engineering and management functions in building life cycle including different types of real estate objects. We think that BIM could not develop separately of LCA. Only their combination can guaranty a new quality and efficiency of construction and real estate.

PROPOSING AN INNOVATIVE ULTRA HIGH PERFORMANCE MORTAR USING RECYCLED STEEL FIBER FROM END-LIFE TYRE AND SPENT CATALYST FROM PETROCHEMICAL INDUSTRY

Hassan Abdolpour

Wroclaw University of Science and Technology, Poland

The research is focused on the recycling of steel fibres and used equilibrium catalyst, which is a waste product of the refinery-based crude oil processing, as a partial substitute of cement in environmentally friendly ultra-high performance self-compacting mortars.

CHEMICAL BIOLOGY & BIOMEDICINE

3D ENVIRONMENT MODULATES PARACRINE ACTIVITY OF STEM CELLS

Olena Rogulska[1,2,3],
Eliška Vavřinová[2], Yuriy Petrenko[1,2]

[1] *Laboratory of Biomaterials and Tissue Engineering, Institute of Physiology of the CAS, Videnska 1083, Prague, Czech Republic*

[2] *Department of Neuroregeneration, Institute of Experimental Medicine of the CAS, Videnska 1083, Prague, Czech Republic*

[3] *Institute for Problems of Cryobiology and Cryomedicine of the NAS Ukraine, Pereyaslavska 23, Kharkiv, Ukraine*

Cell therapy has become one of the most important emerging medical treatments globally. The therapeutic effect of mesenchymal stem cells (MSCs) is attributed mostly to their ability to secrete a wide spectrum of paracrine factors that stimulate the survival and recovery of the resident cells or regulate immune response. The 3D environment is known to have a significant impact on MSC behavior and secretome.

In this study, we aimed to assess the changes of MSC paracrine activity by modulating culture conditions. We compared the viability, proliferation rate, and secretome composition of MSCs cultured in monolayer, scaffolds, simple and composite spheroids. Scaffolds were prepared using cryogelation technique from laminin extract. Simple spheroids were made by hanging drop method, composite ones - generated with the addition of plasma, laminin or collagen using ultralow attachment plates. To evaluate the secretion of bioregulators, Luminex technology was utilized.

In all 3D culture conditions MSCs were viable and metabolically active after 3–7 days of culture. Scaffolds ensured better long-term cell proliferation compared to spheroids. In contrast, the secretion of paracrine factors was dramatically higher in spheroids than in monolayer or scaffolds. Upregulation of FGF-2, HGF, and LIF secretion by MSCs in simple spheroids was >25 fold, while changes in other factors were less prominent. Polymer nature in composite spheroids was also able to affect secretion.

To sum up, the paracrine activity of MSCs can be enhanced by modulating 3D environment likely due to the facilitation of favorable cell-to-cell contact and signaling.

DIALLYL ETHER, A SELECTIVE INHIBITOR OF CYP2E1, PREVENTS INTESTINAL HYPERPERMEABILITY AND ALLEVIATES INFLAMMATION IN *IN VITRO* AND *IN VIVO* MODELS OF COLITIS.

Adam Makaro, Mikołaj Świerczyński,
Agata Grochowska, Maciej Sałaga
Department of Biochemistry,
Faculty of Medicine, Medical University of Lodz

Introduction and aim

CYP2E1 is one of the main members of cytochromes P450 superfamily, which is expressed in numerous tissues, including intestines. Current literature shows that overactivity of intestinal CYP2E1 leads to the loss of intestinal wall integrity and contributes to the development of the leaky-gut syndrome (LGS) which is observed in inflammatory bowel diseases (IBD). It is well-established that the activity of CYP2E1 may contribute to the severity of inflammation due to the production of reactive oxygen species.
The main aim of the study was to evaluate the therapeutic effects of selective CYP2E1 inhibitors in in vitro and in vivo models of intestinal hyperpermeability and inflammation. We used 1) Allyl methyl sulfide, 2) Diallyl ether (DE), 3) Thiophene.

Results

We did not see cytotoxicity of CYP2E1 inhibitors in Caco-2 cells. In the next step, we observed that the permeability of Caco-2 monolayer increased after exposure to fructose, which is one of the main dietary factors responsible for intestinal barrier impairment Caco-2 pretreated with CYP2E1 inhibitors were resistant to those changes. In the following in vitro experiments, DE decreased the level of IL-6 in the culture medium after stimulation of Caco-2 cells with inflammatory cytokines and LPS.
In the in vivo part of the study we evaluated the anti-inflammatory effect of DE in the mouse model of dextran sulfate sodium (DSS)-induced colitis. DE at the dose of 10mg/kg/d p.o. partially reduced macroscopic damage

score of the colon and decreased myeloperoxidase activity. The same dose administered i.c. significantly prevented from the decrease in colon length.

Conclusion

Our experiments show, that CYP2E1 selective inhibitors display beneficial properties. Further studies on these substances may bring additional opportunities to develop novel therapeutics for IBD and LGS.

GENERATION OF REACTIVE OXYGEN SPECIES UNDER THE ACTION OF THIAZOLE DERIVATIVE

Shalai Ya., Ilkiv M., Babsky A.

Department of Biophysics and Bioinformatics,

Ivan Franko National University of Lviv,

Hrushevskyi Str., 4, 79005 Lviv, Ukraine

Reactive oxygen species (ROS) can drive metabolic and mitochondrial dysfunctions, lead to intensive oxidative damage and a tumor-suppressing process (Cheung et al., 2022). Numerous chemotherapeutic drugs that induce oxidative stress in cancer cells have been effectively utilized in clinical settings (Kumari et al., 2018).

The effects of BF-1 (N-(5-benzyl-1,3-thiazol-2-yl)-3,5-dimethyl-1-benzofuran-2-carboxamide), polymeric nanoparticle Th1 and their complex Th2 on ROS production in lymphoma cells were studied. The ROS level was recorded using fluorescence microscopy. The ImageJ software was used to measure and assess the fluorescence intensity.

Statistical analysis of fluorescent images showed, that BF1 and Th2 significantly increased the level of ROS in NK/Ly cells by 27.7% and 28.6% respectively. Meanwhile, polymeric nanoparticle Th1 did not affect the ROS level.

BF1 and its complexes with polymeric nanoparticle significantly increase the ROS generation in NK/Ly cells. Thus, thiazole derivative BF1 may realize its antitumor effect on cancer cells by promoting generation of additional amount of ROS.

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HOW WAR CHANGED PRIORITIES AND VISION IN POCUS EDUCATION

Stanislav Kravchuk

head of Ukrainian POCUS Society

member of Young Talent Group UEG (United European Gastroenterology)

Point-of-Care Ultrasound (POCUS) is a diagnostic ultrasound examination performed by a medical specialist for a quick answer to a specific clinical question. POCUS offers multiple capabilities in a relatively small device to military clinicians of all types in multiple environments.

Since the Russian full-scale invasion of Ukraine in February 2022, ultrasound has become a component of emergency medicine training and POCUS has come to play a vital role in the evaluation of patients by combat medics.

Previous research shows that 4-hour introductory Extended Focused Assessment with Sonography in Trauma (eFAST) training intervention can effectively train conventional military medics to perform the exam to reveal pneumothorax and internal bleeding. Our team of Ukrainian POCUS Society taught 140 military medics to provide ultrasound in trauma and can confirm this data.

We believe that military medics in Ukraine must have the opportunity to master their skills in working with ultrasound machines. Moreover, they should integrate these skills into their work.

STORAGE OF HUMAN MESENCHYMAL STROMAL CELLS IN ALGINATE CAPSULES WITH ADDED PROTEIN

O.S. Hubenia[1,2], S. Leal-Marin[2,3], N.A. Trufanova[1,4], B. Glasmacher[2,3], A. Petrenko[1]

[1] *Institute for Problems of Cryobiology and Cryomedicine of the National Academy of Sciences of Ukraine, Kharkiv, Ukraine*

[2] *Leibniz University Hannover Institute for Multiphase Processes, Hannover, Germany*

[3] *Lower Saxony center for biomedical engineering, implant research and development* NIFE, *Hannover, Germany*

[4] *V. N. Karazin Kharkiv National University, Kharkiv, Ukraine*

Human mesenchymal stromal cells (MSCs) are promising cell type for biomedical research and clinical medicine. Cell storage at ambient temperatures may simplify transportation and overcome disadvantages of cryopreservation. Here we study the cell cycle, viability, metabolic activity of MSCs during storage at ambient temperature in five different forms: monolayer, suspension, encapsulation in alginate capsules (AMS), and AMS with addition of fresh porcine blood plasma or human amniotic membrane (hAM) extract. The extract was obtained from hAM after dissection of the placenta, followed by freeze-drying and membrane digestion. The experiments were performed on human bone marrow MSCs provided by Clinic for Orthopedic at Hannover Medical School and cultured in sealed containers at 22 °C alfa-MEM supplemented with 10% (v/v) of fetal bovine serum. Alginate 2.5% (w/v) low-viscosity was used for the AMS production. The protein concentration of AMS with hAM extract or porcine blood plasma was standardized (BCA Protein Assay Kit, Bradford Assay) to 32.6 µg/ml. Viability (Trypan Blue, FDA/EthD dual staining), metabolic activity (Alamar blue) were assessed on 1, 3, 5 and 7 days of storage. For cell cycle analysis, MSCs were transduced with the Premo™ FUCCI Cell Cycle Sensor, then cultured in monolayer or AMS and live-cell imaging of cell cycle progression with confocal laser scanning microscope Olympus FV10i-LIV with Olympus cellSense Software.

The findings indicated that the metabolic activity of cells in AMS decreased by 40% after 1 day of culture, as opposed to MSCs cultured in a monolayer. AMS with the addition of hAM extract, or porcine blood plasma decreased to 52% and 45% compared to MSCs in monolayer, respectively. Viability assessed by FDA/EthD decreased 70% during MSCs storage in monolayer, 40% in suspension, 87% in AMS with hAM extract, and 62% with porcine blood plasma at day 7 compared with initial viability after day 1. Metabolic activity follows a similar decrease trend on the same days. On the other hand, at day 7 AMS without hAM or plasma presented viability of 85% and metabolic activity of 55% from initial indexes. Furthermore, AMS with hAM extract and porcine blood plasma had metabolic activity of 53% and 62% of initial indexes, correspondingly. Cell cycle analysis showed that MSCs were completely arrested in G1 phase 2 days after encapsulation.

The benefits of AMS for the MSCs short-term storage and transportation under ambient temperature were shown with a correlation between the decrease of cell metabolic activity and cell viability.

HYDROXYL RADICAL FORMATION AND DNA DAMAGE UNDER CONVENTIONAL AND ULTRA-HIGH DOSE RATE ELECTRON RADIATION

Y. Komar[1], A. Grebinyk[1,2], M. Frohme[1],
Z. Aboulbanine[2], N. Aftab[2], Z. Amirkhanyan[2],
A. Asoyan[2,3], H. Davtyan[2,3], D. Dmytriiev[2],
G. Georgiev[2], M. Gross[2], A. Hoffmann[2],
M. Krasilnikov[2], X. Li[2], M. Liebel[2],
G. Loisch[2], Z. Lotfi[2], A., A. Oppelt[2],
C. Richard[2], F. Riemer[2], F. Stephan[2],
H. Qian[2], G. Vashchenko[2]

[1] *Technical University of Applied Sciences Wildau, Division Molecular Biotechnology and Functional Genomics, Wildau, Germany,*

[2] *Photo Injector Test Facility, Deutsches Elektronen-Synchrotron, DESY, Zeuthen, Germany*

[3] *on leave from CANDLE Synchrotron Research Institute, Armenia*

In Germany, 50-60% of cancer patients are being treated with radiation therapy. Ionizing radiation causes indirect and direct DNA damage during radiolysis of water, inducing reactive oxygen species production and DNA damage. The Photo Injector Test facility at DESY in Zeuthen (PITZ) together with Technical University of Applied Sciences Wildau provides a unique platform FLASHlab@PITZ with an electron beam delivered at both conventional low (LDR) and ultra-high dose rate (UHDR). The aim of this study is to evaluate DNA damage (single and double strand breaks, SSB and DSB) and hydroxyl radical level after UHDR and LDR irradiation in water.

The 22 MeV electron beam delivered ≤60 Gy doses at 0.05 and 105–106 Gy/s. The formation of hydroxyl radical was measured by its reaction with coumarin. The amount of SSB and DSB in the DNA plasmid pBR322 formed after irradiation was evaluated with agarose gel electrophoresis. The yield of DNA plasmid pBR322 isoforms was estimated with the McMahon and Currell approach.

Generation of hydroxyl radicals was observed in a dose-dependent manner at the doses of ≤60 Gy. SSB and DSB were quantified at doses ≤50 Gy. Higher level of hydroxyl radicals was observed with LDR radiation as with UHDR whereas no significant difference was observed between isoforms of DNA plasmid pBR322 irradiated with UHDR and LDR.
The observed data characterized the initial biochemical effects of ionizing radiation at UHDR that pointed on a high potential for the development of cancer UHDR electron radiotherapy at FLASHlab@PITZ.

DIGESTIVE HEALTH RESEARCH IN LODZ, POLAND

Maciej Salaga

Department of Biochemistry, Medical University of Lodz, Poland

"We are what we eat" is a common saying, yet not always understood and applied. On the other hand, the gastrointestinal (GI) tract has emerged as a crucial system, intertwining structurally and functionally with the central and peripheral nervous as well as immune systems. Therefore, not only diet, but also lifestyle and surrounding environment may influence the digestive health. Irritable bowel syndrome (IBS)-related examination constitutes 25–50% of the entire gastroenterology outpatients workload and the incidence of inflammatory bowel disease (IBD) is estimated at 5 per 100,000 people per year and the prevalence is 40–50 per 100,000 people in the Western and Northern Europe. The field of GI research is steadily growing worldwide in recent decades which is also reflected in Poland. Department of Biochemistry at Medical University of Lodz is one of the leading polish research centers that specializes in investigating the pathophysiology of functional and inflammatory diseases of the GI tract. The main aims of our studies are (i) to understand the pathophysiology of gastrointestinal diseases and the involvement of intrinsic and extrinsic factors (opioid, cannabinoid, serotonin, and orphan receptors), (ii) to validate new pharmacological targets for future treatment of IBS and IBD and (iii) to design and test novel molecules with therapeutic potential in the GI tract. In or work we use intestinal cell line cultures, colonoids and immune cell cultures. In vivo methods that we use are animal models of functional gastrointestinal disorders: intestinal motility tests, abdominal pain. Models of inflammatory diseases: gastric ulcer, IBD (ulcerative colitis, Crohn's disease) both acute and chronic, colorectal cancer associated with inflammation, type 2 diabetes.

THE NEGATIVE EFFECT OF AMINO ACIDS ON THE EXOCRINE PANCREAS IS ASSOCIATED WITH THEIR CATABOLISM IN MITOCHONDRIA

Zub A.M., Manko B.O., Manko V.V.

Human and Animal Physiology Department

Ivan Franko National University of Lviv

Hrushevskyi Str., 4, 79005 Lviv, Ukraine

Mitochondrial damage is the main event in the development of amino acid-induced acute pancreatitis (Biczó et al., 2011; Biczo et al., 2018). We hypothesized that the effects of amino acids on the pancreas can be caused by metabolic pathways in mitochondria. The aim of our study was to find out the effect of amino acids on energy processes and the viability of rat pancreatic acinar cells.

Experiments were carried out on male Wistar rats. A suspension of isolated pancreatic acini was obtained using collagenase. The rate of oxygen absorption was recorded by the polarographic method. Cell viability was assessed by fluorescent microscopy using ethidium bromide and Hoechst 33258.

We found that glutamate, glutamine, alanine, lysine and aspartate significantly stimulated uncoupled mitochondrial respiration. Asparagine, arginine and histidine did not change oxygen consumption by mitochondria of pancreatic acinar cells. A significant increase of cell blebbing was detected after 2 and 4 h incubation with glutamine and only after 2 h—with aspartate. Glutamine caused cell swelling after 2 and 4 h of incubation. After 24 h of incubation, only alanine and histidine did not decrease the viability of pancreatic acini. Glutamate, asparagine and aspartate displayed moderate toxicity, while lysine, arginine and glutamine caused complete loss of cell viability.

In conclusion, this study partially demonstrates a correlation between the ability of pancreatic acinar cell mitochondria to oxidize amino acids and their toxicity in these cells. The negative effect of lysine and glutamine on cell viability is probably realized in different ways, but it may be related to the formation of metabolites during the catabolism of these amino acids.

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QUANTUM PHYSICS & CHEMISTRY

CONTROLLING CHEMISTRY WITH CAVITY QUANTUM ELECTRODYNAMICS

Felipe Herrera

Universidad de Santiago de Chile, Chile

Modifications in reaction rates for chemical processes have been reported to occur in infrared cavities due to strong coupling between the vibrations of reactant molecules and the cavity vacuum [1,2]. However, there is currently no consensus on the microscopic mechanism enabling these observations. an open quantum system approach is employed to model recent experiments on the alcoholysis of phenyl isocyanate (PHI) with cyclohexanol monomers in a liquid-phase Fabry-Perot cavity [3]. The focus is on the resonant suppression of the NCO stretching mode of PHI molecules due to strong vibrational coupling at normal incidence with one of the cavity modes.
Taking into account inhomogeneous broadening, cavity photon losses, intramolecular vibrational coupling, vibrational relaxation, thermalization, and many-particle effects, this study demonstrates that stationary resonant modifications of chemical reactivity within a molecular ensemble are possible via light-matter quantum coherences. This suggests fundamental links between chemistry and quantum science that can be further explored at room temperature.

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MULTIBRAND FLATTENING AND LINEAR DIRAC BAND STRUCTURE IN GRAPHENE WITH IMPURITIES

Somayeh Ahmadkhani

Nicolaus Copernicus University in Toruń, Poland

Flat bands in the energy spectrum have garnered significant attention in recent years due to their unique characteristics and promising applications [1]. Researchers have proposed a special arrangement of impurities on monolayer graphene to generate multi flat bands in its electronic band structure. When studying graphene with low hydrogen density, we observed single mid-gap states in the spectrum [2]. However, with increasing impurity density, we discovered closely spaced bands around the Fermi level, resembling discrete lines similar to those found in the spectrum of quantum dots. This phenomenon also shares similarities with the unusual Landau-level energy spectrum observed in graphene subjected to a strong magnetic field [3].

The existence of flat bands is highly dependent on whether there are odd or even electrons of H(F) atoms bound to graphene. Interestingly, a fully hydrogenated (or fluoridated) hexagon of a graphene sheet, with six hydrogen (or fluorine) atoms placed on the top and bottom in consecutive order, exhibits Dirac cones in the electronic band structure. These Dirac cones have a 20% smaller Fermi velocity compared to pristine graphene. Functionalizing graphene introduces various C-C bond lengths, leading to nonuniform strains in the material. This nonuniform strain can induce a giant pseudomagnetic field, resulting in a quantum Hall effect in the system [4].

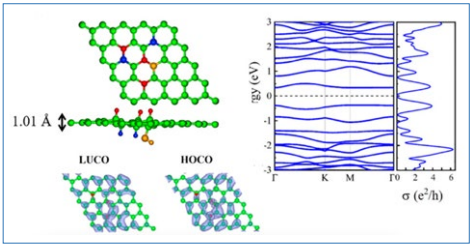

Figure 1: Calculated mutual information between constituent atoms of Tyrosine-Glycine dipeptides.

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ADVANCED AB INITIO CALCULATIONS AND CHEMICAL REACTIONS STUDY OF ULTRACOLD ALKALI-METAL AND ALKALINE-EARTH-METAL DIATOMIC MOLECULES

Hela Ladjimi

University of Warsaw, Poland

We study the energetics of chemical reactions between ultracold, ground-state alkali-metal and alkaline-earth-metal diatomic molecules. We show that the atom-exchange reactions forming homonuclear dimers are energetically allowed for all heteronuclear alkaline-earth-metal combinations. We perform high-level electronic structure calculations on the potential energy surfaces of all possible homo- and heteronuclear alkaline-earth-metal trimers and show that trimer formation is also energetically possible in collisions of all considered dimers. Interactions between alkaline-earth-metal diatomic molecules lead to the formation of deeply bound reaction complexes stabilized by large non-additive interactions. We check that there are no barriers to the studied chemical reactions. This means that all alkaline-earth-metal diatomic molecules are chemically unstable at ultralow temperatures. Optical lattice or shielding schemes may be necessary to segregate the molecules and suppress losses.

HOW CAN ONE CHEAPEN THEORETICAL BENCHMARK VALUES FOR TRANSITION METAL-CONTAINING COMPOUNDS?

Matheus Morato Ferreira de Moraes

Federal University of ABC (UFABC), Brazil

Although relevant in a wide range of experimental fields, the reliable modeling of transition metal-containing compounds is a known challenge. The necessity to account for a large number of effects, derived mainly from the partially filled d-shell, drastically increases the computational cost scaling with the system size, which prevents the use of the usual methodologies applied in systems composed only of representative atoms. Among the highest accurate theoretical methods able to model these systems, multireference wave function (MR-WF)-based ones are usually required, especially when the system's interest lies in its excited structure [1]. Despite their high accuracy, these methods have a main setback when applied to first-row transition metal-containing compounds: the presence of the double d-shell (or 3d double-shell) effect [2]. The usual protocol to include this effect makes the use of MR-WF-based methods infeasible even for diatomic systems, due to its unfavorable computational cost scaling.

On the other hand, the lack of this effect leads to large errors in the relative energies among states and, in some cases, in the qualitative character of the ground state wave function [3]. In this presentation, an alternative definition for the double d-shell effect, the multi-d-occupancy character of the wave function, will be explored. Moreover, we are going to show that based on this definition, it is possible to develop a protocol able to cheapen MR-WF calculations for systems that depend on this effect without a substantial loss of accuracy [4].

With the further development and validation of this, or a similar, approach, the application of highly accurate MR-WF-based methods shall become substantially cheaper to model first-row transition metal-containing compounds' ground and excited electronic structure.

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THE LOW-LYING EXCITED STATES OF LIYB+

Marta Gałyńska

Nicolaus Copernicus University in Toruń, Poland

Quantum chemistry encompasses a diverse range of methods that hold the power to predict all essential properties associated with atoms and molecules' ground and lowest-lying excited states, specifically at absolute zero temperature. Recent advancements in laser cooling techniques have opened up new possibilities for experimental investigations into compounds in their electronic ground state. Over the past two decades, sophisticated experimental methods have been extensively employed to delve into the chemistry and physics of cold and ultracold atoms as well as molecules, typically within the temperature range of 1.0 mK to 1.0 K. These groundbreaking experiments enable precise measurements of atoms or molecules by skillfully manipulating their specific quantum states.

Among the elements, ytterbium stands out as an incredibly valuable asset owing to its closed f-shell and ground-state electronic configuration of $4f^{14}6s^2$, which closely resembles that of group II atoms. However, ytterbium, with its 70 electrons, falls under the category of heavy elements. Heavy elements pose an exceptional challenge to modern quantum chemistry due to the significant impact of spin-orbit coupling (SOC) effects and the large number of correlated electrons involved in calculations. Nevertheless, in many investigations of ytterbium compounds within quantum chemistry, the effects of spin-orbit coupling are often overlooked due to the computational expense associated with incorporating them. in this study, we delve into the influence of relativistic effects on the low-lying excited states of LiYb+ by utilizing the Equation of Motion CCSD method.

THEORETICAL STUDY OF THE ELECTRONIC STRUCTURE AND PROPERTIES OF POLYANILINES FROM MODERN QUANTUM CHEMISTRY

Seyedehdelaram Jahani

Nicolaus Copernicus University in Toruń, Poland

Since the discovery of conductive polymers, polyanilines have found a wide range of applications, including in life sciences, electronics, photovoltaics, solar cells, and sensors [1]. We employ state-of-the-art quantum chemistry methods to investigate the structure-to-property relationship in polyanilines (PANIs) of different lengths and oxidation states. Specifically, we focus on leucoemeraldine, emeraldine, and pernigraniline in their tetramer and octamer forms. Our scrutiny includes an analysis of their structural properties, HOMO and LUMO energies, HOMO-LUMO gaps, as well as vibrational and electronic spectroscopy, using various Density Functional Approximations (DFAs). Furthermore, we assess the accuracy of DFAs by comparing them to experimental and wavefunction-based reference data [2].

Our study is augmented with quantum entanglement and orbital correlation analysis [3] from large-scale orbital-optimized pair-Coupled Cluster Doubles (oo-pCCD) calculations [4], considering both ground and electronically excited states [5]. These calculations are performed using the PyBEST software package [6].

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BENCHMARKING IONIZATION POTENTIALS FROM THE SIMPLE PCCD MODEL

Saddem Mamache

Nicolaus Copernicus University in Toruń, Poland

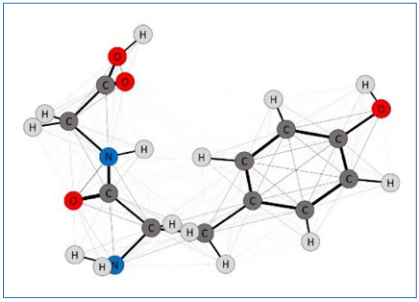
The electron-detachment energy is measured by its ionization potential (IP). As a result, it is a fundamental observable and an important molecular electronic signature in photoelectron spectroscopy. A precise theoretical prediction of electron-detachment energies or ionization potentials is essential for organic optoelectronic systems such as transistors, solar cells, or light-emitting diodes. In this work, we benchmark the performance of the recently presented IP variant of the equation-of-motion pair coupled cluster doubles (IP-EOM-pCCD) model to determine IPs. Specifically, the predicted ionization energies are compared to experimental results and higher-order coupled cluster theories based on statistically assessing 201 electron-detached states of 41 organic molecules for three different molecular orbital basis sets and two sets of particle-hole operators. While IP-EOM-pCCD features a reasonable spread and skewness of ionization energies, its mean error and standard deviation deviate up to 1.5 eV from reference data. Our study thus highlights the importance of dynamical correlation to reliably predict IPs from a pCCD reference function in small organic molecules.

EXPLORING MOLECULAR BONDING THROUGH MUTUAL INFORMATION: A QUANTUM INFORMATION APPROACH

Mostafa Javaheri Moghadam,
Stijn De Baerdemacker
University of New Brunswick, Canada

Proteins, as essential biomolecules, play diverse roles in biological processes. Understanding the intricate structure and function of proteins requires a comprehensive study of their constituent building blocks: the amino acids. These 20 naturally occurring amino acids combine in various sequences to form the primary structure of proteins, which, in turn, dictates their tertiary functional configuration. Although accurate descriptions of amino acid interactions necessitate high-quality ab initio methods, these techniques are often limited to medium-sized systems. As a result, exploring larger systems typically relies on less sophisticated methods like force fields and molecular dynamic simulations, which lack the quantum correlation energy contribution and may lead to inferior accuracy.

In this study, we introduce the concept of quantum mutual information as a means to comprehend the chemical interactions of amino acids. Our analysis revolves around the entanglement between pairs of atomic orbitals situated within the encompassing environment of all other active-space orbitals. By employing von Neumann entropy and a one- or two-particle reduced density matrix [1], we assess the orbital entropy and atomic mutual information across a variety of dipeptides. Our findings demonstrate that atomic mutual information represents a valuable tool for gauging the strength and character of chemical bonding in biomolecules. Through the examination of these metrics, potential interactions between amino acids are uncovered, thereby expanding their applicability to larger systems.



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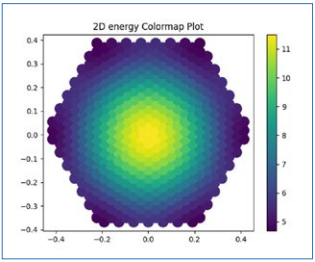
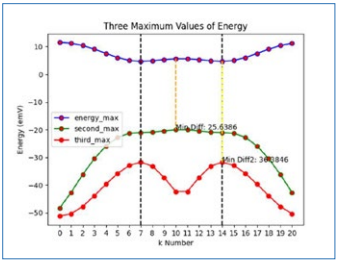
TRIANGULAR LATTICE HUBBARD MODELS ON TMD

Saman Behjou
Paweł Potasz
Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Toruń, Poland

In this research, we have focused on investigating the Hubbard model on a triangular lattice in two-dimensional materials (TMDs). The Graphene is just one example of a large class of two-dimensional crystals [1]. These crystals can either be extracted from layered three-dimensional materials or grown artificially by several different methods [2]. The Hubbard model is a mathematical model used in condensed matter physics to describe the behavior of interacting electrons in a solid-state material [3]. we are working on Triangular Lattice in Real Space and Reciprocal. In this case, we have meshed the central points of the hexagonal cells in the lattice at exactly equal and periodic intervals, so that our selected mode point is always in the center of the meshing, and the ends of the meshing form our hypothetical boundaries. we construct Moiré band Hamiltonians for holes in twisted heterobilayers formed from semiconducting transition metal dichalcogenides (TMDs), Considering that the meshing can include an infinite number of k points, but considering that a value greater than 400 does not affect the results of the calculations and is the same.





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QUANTUM EMBEDDING WITH PAIR COUPLED CLUSTER DOUBLES-BASED METHODS

Rahul Chakraborty

Nicolaus Copernicus University in Toruń, Poland

Reliable quantum-chemical modeling of large molecular systems still remains an elusive question. Wave function theory (WFT)-based methods, although highly accurate, are limited by very high computational scaling. Quantum embedding methods have shown promising results in addressing this challenge. In this approach, the molecular structure is partitioned into a system part studied by more reliable WFT methods, and the environment part is modeled by low-level methods. We propose a novel embedding scheme, augmenting pair-coupled cluster doubles (pCCD)-based methods as the WFT-based component for the system fragment with density functional theory (DFT) approximations for the environment.

The pCCD method produces reliable results for strongly correlated systems with mean-field computational scaling. We also use a posteriori linearized coupled cluster (LCC) corrections on the pCCD wave function to account for the large extent of dynamic correlation, missing in the pCCD ansatz and its extension to excited states. All codes have been implemented in the developer version of the PyBEST software package.

We have tested our embedding methods for the water-ammonia complex and, for a more challenging task, uranyl halides. The accuracy of the proposed model is assessed against the vertical excitation energies and orbital correlation analysis. Our work serves as a starting point for further development of pCCD-based embedding schemes.

INTERDISCIPLINARY RESEARCH IN HUMAN SCIENCES

ONE YEAR OF WAR IN UKRAINE: IMPACT ON ENERGY AND ENVIRONMENT

Galyna Trypolska

SO „*Institute for Economics and Forecasting*, UNAS", *Ukraine*

Institute for Rural and Agricultural Development,

Polish Academy of Sciences, Poland

The full-scale invasion of russian federation in Ukraine that began on Feb 24th, 2022 and lasts until now, has resulted in the numerous losses for Ukraine's economy and human capital. Ukraine witnessed a 30% GDP decline, and the temporary loss of more than 8 million people, mostly women and children, who fled from war abroad. The war brought to Ukraine significant deterioration of the environment, caused by numerous shelling, use of prohibited weapons, fires due to shelling, including in Chornobyl forests, and the need for demining half of the territory of Ukraine. There is unprecedented infrastructure destruction. Energy and environment are the areas that experienced the highest losses, as destruction of Ukraine's energy infrastructure is one of the tools to force Ukraine to stop fighting. The overall damage to energy of Ukraine after one year of a full-scale war equaled USD 8.1 billion.

PROBLEMS OF SALT PRODUCTION AND TRADE IN PRE-INDUSTRIAL EASTERN EUROPE

Monika Kaminska

Independent researcher, Poland

My current scientific interests focus on the problems of salt production and trade in pre-industrial Eastern Europe (mainly on the territories between the Eastern Carpathian and the Black Sea regions). The investigation of medieval and post-medieval salt works, mines, salt markets, and tolls requires a multidisciplinary approach. Since the "white gold" remains one of the least material of the material commodities of humankind, the history of its exploitation, the trade routes, and different elements of salt-related culture (e.g. tableware) can be only reconstructed by the use of different types of sources and literature from the scientific fields of the geology, history, archaeology, cartography, linguistics and even history of art. The aim of the project is to create as coherent and transparent a picture as possible of the history of salt production and trade in the area of the study, showing the trade routes and means by which salt reached the tables of people living outside the salt-bearing areas. An important element of the work is the recording of all the elements of material culture heritage associated with one of the most intangible, in retrospect, goods of mankind. I will try to provide a draft of the study on salt circulation between Slav and Nomad worlds of medieval and Early Modern Period Eastern Europe during my short presentation.

HUMANS IN DIGITAL WORKPLACE: THE CASE OF EUROPEAN WAREHOUSING

Aneta Pieczka

Kozminski University, Poland

Are machines and digital technologies taking control over humans in the workplace?

This study answers this question, responding to the rapid advancement of technology. Using a case in warehousing sector, highly reliant on automation, robotics, and data-driven systems, I study how technological advancements shape the employee experience.

Current literature focuses on efficiency. It means that integration of technology in warehousing operations, for most scholars means that technology boosts productivity while reducing costs and time of processing. However, the relationship between digital technologies and human factor in warehouses remains limited.

To answer this gap, I am study European warehousing sector, working in a collaborative project HuLog (Humans in Digital Logistics). HuLog relies on a multiple-case research of 12 European warehouses (Poland, Belgium, Germany and UK) and will produce multidisciplinary, cutting-edge scientific knowledge on work and employment in European logistics.

My role in answering these questions is concentration on the meaning of technology adoption and understanding the study of meaning of algorithmic, technological work from multiple perspectives of a warehouse organization. This niche, which I address in my work, has a tremendous potential in assessing subjectivity of a worker exposed to all-encompassing technology. The questions of this positionality will soon need to be addressed not only in social sciences but also in law and policy-making.

At the culmination of the project, besides academic outputs, recommendations will be formulated for companies facing the challenges of digital transformation.

THE CONTEMPORARY HUMAN CONDITION IN THE CONTEXT OF JÓZEF TISCHNER'S PHILOSOPHY OF DRAMA

Paweł Nowak

Nicolaus Copernicus University in Toruń, Poland

During the speech, I will present the subject of my doctoral thesis—the contemporary human condition in the context of Józef Tischner's philosophy of drama. I will present the methodology of my work and talk about the first conclusions from the research. The philosophy of man, in which Tischner's philosophy undoubtedly fits, has a very important role to play during great transformations and crises. The values presented by the philosophy of drama can become a valuable indication for a modern man who often loses the support of his humanity, gets lost in the maze of ideology and loses himself in consumerism.

INVISIBLE INEQUALITIES AGAINST WOMEN FROM THE UPPER SOCIAL STRATA

Wiktoria Morawska

Institute of Philosophy and Sociology,

Polish Academy of Sciences, Poland

The aim of the lecture is to analyze inequalities in social allocation due to gender in the lives of young, advancing women: professionals and entrepreneurs. Women from this group internalize the social structure and have an ambivalent attitude towards the implementation or the attempt to reject gender roles. This tension—what I call invisible inequalities—may be a fundamental source of further perpetuation of gender inequalities, which is especially evident in this research group that theoretically has all the resources to make equality possible.

The speech will be a presentation of the results of research conducted using the technique of 32 biographical interviews, analyzed using MAXQDA. In my speech, I will talk about the autonomy of gender structures in relation to the changing legal and economic structures in the context of the image of a contemporary Polish woman.

THE REACTION OF THE MEDICAL COMMUNITY TO THE TIGHTENING OF ABORTION LAW IN THE WORLD ON SELECTED EXAMPLES

Nikola Lewicka

University of Silesia in Katowice, Poland

In Chile, in the 1970s, the topic of abortion was pushed to the background by feminist movements. The only chance to change the then strict law came from members of the medical community. At Santiago's Barros Luco Hospital, a team of obstetricians and gynecologists began performing abortions on the basis that they were "therapeutic" because women would not seek unsafe termination methods and therefore would not be at risk of a health complication or even death. It is estimated that only from March to September 1973, about 3,000 abortions were performed in this hospital.

This is not the only case where the medical community has had a key relationship with subsequent law reform. Examples from other parts of the world can be found in the United States or Ghana, where initially only individuals broke restrictive regulations, risking imprisonment or loss of the right to practice. Soon, other doctors also began to support "civil disobedience", which influenced professional organizations to take political action to reform the abortion law.

According to the World Health Organization, approximately 25 million abortions take place each year that are not performed under safe conditions, and each one poses a health risk to the person performing it. In a situation where human health and life are at stake, can we consider abortion a legal issue, disregarding health advocacy? If not, can a heroic attitude be expected from anyone, especially if it may have consequences for that person?

In my speech, I will draw attention to the role of medics and their impact on changes in the abortion law.

Based on the experience gained at the CEDAW Committee at the United Nations, I will focus on selected examples from around the world and on individuals who have had an impact on change.

UN ON THE CIVIL WAR IN YEMEN: IMPLEMENTATION OF THE RESPONSIBILITY TO PROTECT DOCTRINE?

Karolina Siekierka

UN Global Compact Network Poland, Poland

The responsibility to protect principle was adopted by the international community during the 2005 World Summit. It is based on three pillars: (i) the responsibility of each State to protect its populations, (ii) the responsibility of the international community to assist States in protecting their populations, (iii) the responsibility of the international community to protect civilians when a State is failing to do so. These principles are deeply embedded in international law, as states have to prevent and punish crimes of genocide, war crimes, ethnic cleansing, and crimes against humanity. States, however, implement the principle selectively, depending on their interests. And although it is not difficult to find publications on the responsibility to protect principle, there is no literature discussing this issue in the context of the Yemeni civil war, which began in 2015. Nonetheless, the situation in Yemen constitutes a threat to international peace and security.

The intervention of neighboring states contributed to the intensity of the conflict, as well as to a significant increase in the number of civilian casualties. Global powers (USA, UK, France, etc.) are indirectly related to the conflict.

INNOVATION IN THE GLOBALIZED WORLD: DISPARITIES, UNEVENNESS, & CHALLENGES

Stefaniia Parubets

Kyiv National Economic University named after Vadym Hetman, Ukraine

In today's globalized world, there is a lack of uniformity in the distribution of innovation capacities, resulting in unevenness in innovative development. This situation is characterized by certain regions and countries possessing greater innovation capabilities, while others lag. The focus of the study is to investigate the underlying nature and structure of these asymmetries in innovative development. By utilizing various indicators of innovative development, it is possible to identify leading countries that form innovative enclaves, while other states, primarily lower-middle-income developing countries, strive to catch up with these innovation frontiers. Distribution of innovation capacities is uneven creating a situation of asymmetry of innovative development: certain regions and countries have a greater capacity for innovation, while others lag behind. The asymmetries in innovation represent a complex and multifaceted paradigm of unevenness in innovative development. Policymakers must take proactive measures to foster innovation, reduce disparities, and ensure sustainable and equitable global development. Asymmetries of regional innovations can be characterized by certain regional leaders: North America, Europe and Central Asia and East Asia, and the Pacific. These regions are the leaders due to the presence of countries-leaders of innovative development, mainly the USA, EU countries, China, Japan, and South Korea. Regional outsiders are Sub-Saharan Africa, South Asia, Latin America, and the Middle East. Asymmetries of global innovations are characterized by countries with high incomes having better indicators of innovation, however, countries with high incomes are not clear-cut leaders in all innovation indicators. Additionally, countries with incomes above the average are actively developing in the innovation sphere and, can become leaders in innovative global development. At the same time further innovation development in Ukraine is dependent on the implementation of the principle of an innovative partnership to reduce the fragmentation of efforts between interested parties; strengthen the means of supporting innovation using the possibility of involvement in EU structural funds and programs; simplify administrative procedures to facilitate access to financing; stimulate the formation of partnerships and connections between education, business, science, and innovation; stimulate entrepreneurship by supporting young innovative companies.

THE RUSSIAN-UKRAINIAN WAR IN EUROPEAN CONTEXT

Olesia Zvezdova

Petro Mohyla Black Sea National University, Ukraine

Augsburg University, Germany

The events, currently taking place in the world, indicate that population of Europe continent is on a verge of transformations in the field of international security, including psychological security as well. Throughout the Russian-Ukrainian hybrid war (since 2014), Russian Federation actively continues to use different psychological mechanisms of influence on the population of Ukraine, European Union and even its own population. It is proposed to focus at five main mechanisms of Russian psychological influences in Ukraine that are divided according to the means of information dissemination.

MY CASE OF EARLY MODERN POLISH-LITHUANIAN PARLIAMENTARISM HISTORY STUDYING: THE SEJMIK OF CHERNIHIV VOIVODESHIP IN THE REIGN TIME OF WETTINS (1697–1763)

Yevhen Shymanskyi

History of Ukraine Department,

Borys Grinchenko Kyiv University, Ukraine

The author reveals the essence of his study of the phenomenon of noble parliamentarism of the early modern state of the Polish-Lithuanian Commonwealth on the Ukrainian lands. The topic covers the political activity of the nobility at the Sejmik of the Chernihiv Voivodeship in exile, which was held in Volodymyr. The chronology covered by the author in his research is the period of Interregnum after the death of King Jan III Sobieski (1696–97) and the so-called era of the Saxon Wettin dynasty (August II and August III)—1697–1763 (the main topic). The author describes the goals and methods of studying the instrumentality of this sejmik in the hands of political factions and also shows the state of the source base—Sejmik acts, one part of which is located in Kyiv (Central State Historical Archive in Kyiv) and Warsaw (Central Archives of Historical Records in Warsaw), and the other is published in the early 20 th century (Acts of Southern and Western Russia). The author also expresses the need to unify and publish the Sejmik acts of the Chernihiv Voivodeship. Finally, the author outlines his plans for research based on Warsaw archives and libraries and briefly reviews his last historical articles on the topic of the Interregnum after the death of Jan III Sobieski.

INSTRUCTIONS TO AMBASSADORS TO THE DIET AS A SOURCE OF THE EXTERNAL AND INTERNAL SITUATION OF THE POLISH-LITHUANIAN COMMONWEALTH BASED ON THE EXAMPLE OF THE SOURCES OF THE RUTHENIAN VOIVODESHIP 1669–1696

Marta Znak

Faculty of History, Ivan Franko National University of Lviv, Ukraine

Pre-sejm sejmiks belonged to the oldest noble assemblies. Pre-sejm sejmiks were convened by the king. The monarch sent special documents (universal and royal instruction) to each sejmik, outlining the reasons the next Diet would be held. Such sejmiks elected one to six ambassadors, who represented the interests of a specific noble assembly. In the Ruthenian Voivodeship, during the period under study, two provincial sejmiks were held in Kholm and Halych (for the local nobility) and one "General" sejmiks in Vyshnia (for the Lviv, Peremyshyl, Sanok lands).

The nobility drew up instructions for ambassadors at the pre-sejm sejmiks. Ambassadors were given instructions on how to vote during the Diet proper, although on occasion the instructions could be vague, or even give the deputies complete freedom. The content of the instructions to the ambassadors was related to the content of the royal instructions. The royal instructions informed the nobility about the issues and problems that will be discussed at the Diet.

The purpose of this study is to analyze which domestic and foreign policy issues Polish–Lithuanian Commonwealth are considered in the instructions to ambassadors to the Diet. The source of this research is the instructions of the Ruthenian Voivodeship 1669–1696. From the analyzed sources, we can separate three thematic groups of issues: 1. general 2. local. 3. private.

The Polish-Lithuanian Commonwealth had a centralized structure, so all important issues of domestic and foreign policy were decided by the Diet. The general group includes finances (taxes, treasure and other financial matters); activities of state institutions (the Diet, the Crown tribunal and others); the army; wars and signing peace treaties; foreign policy; religious issues; ennoblement and others.

The next group includes issues of a local nature that related to a specific voivodeship or land. Such questions could be presented as in the royal instructions and fit in at the initiative of the nobility itself. The next group includes issues of a private initiative of the nobility. The nobility often tried to solve private property problems with the help of the Diet.

ON THE QUESTION OF PRESERVING THE HERITAGE OF ZAWISZAS

Kseniya Liubaya

University of Warsaw, Poland

Zavishy is a noble family closely connected with the history of the lands of Central and Eastern Europe for five centuries. The first information about Zavishy is related to the reign of Grand Duke Kazimierz Jagielonczyk (middle of the 15th century), the last ones relate to the Belarusian national revival of the beginning of the 20th century. Unfortunately, if we turn to the historiography of the Zavyshas, we will find that the works dedicated to this family are mainly of a popular literature. Therefore, this topic is of interest to me as a beginner researcher.

The legacy of Zavishy is at a disadvantage. In 2022, a part of the Zavishas estate in Pershamaisk, which currently belongs to Uzda State College, was put up for sale. Also, the collection of portraits of Zavishy was divided between three countries.

My project will be dedicated to the problems of preserving the material heritage of Zawishy. As well as the possibility of creating a site-museum of Zawiszas.

THE MEDIEVAL HISTORIAN'S WORKSHOP IN REFERENCE TO THE VOYAGE OF SOPHIA OF LITHUANIA TO MOSCOW IN 1391

Adrian Kryszak

Nicolaus Copernicus University in Toruń, Poland

The primary purpose of this lecture is to introduce the workshop of a historian concerned with the medieval political history of Rus' and introduce their research methodology and what they have to face. A presentation based on a short example based on the issue of Sophia of Lithuania (1371–1453), voyage to Moscow for a wedding ceremony with Vasily I Dmitriyevich. This example is intended to show how important each detail is in studying history, and what we can conclude from the correctly reconstructed travel route.

PLANTS, APPEARANCES AND THE CRISIS OF INSCRIPTION AT AUSTERLITZ BY W. G. SEBALD

Noemi Szafrańska

Jagiellonian University in Cracow, Poland

The purpose of the paper is to analyze W. G. Sebald's novel „Austerlitz", in which the reflection on the condition of literature in the era of late postmodernity is present. The central issue for this reflection turns out to be the clash between the notion of appearances and plants. At the outset, the author invokes a quotation from Parmenides' poem "On Nature" and Franz Kafka's "Trees" by Franz Kafka, thus outlining the characteristic way of defining the epistemological value of appearances and plants in Western philosophy. Analyzing W. G. Sebald's novel in this context, she points out the important role of the association of plant motifs with highly exploited literary topoi in the text. In particular, the ironic play with the interpretation of human anatomy in the spirit of humanistic affirmative anthropology, Calderón's juxtaposition of stars and flowers and the motif of living a dream are discussed. In the last part of the paper, the author presents the specifics of the novel's narrative, interpreting how it works in the context of the analyses conducted earlier. Austerliz proves to be a text that shows literature as an excellent tool for staying in the most cognitively authoritative movement of disillusionment, apprehension and further illusions while diagnosing the crisis of inscription.

"MEN'S WORLD" OF NOBLE FAMILIES OF THE KYIV PROVINCE (1793–1917)

Anton Tereshchuk

Uman State Pedagogical University, Ukraine

The topic of my research is: "Men's world" of noble families of the Kyiv province (1793–1917). My supervisor is Professor Ihor Kryvosheya—a professor at Uman State Pedagogical University, and a leading specialist in the 19th-century history of Ukraine and the Polish nobility.

The research involves the analysis and study of the daily life of men of noble families, that is, the reproduction of the pattern of their everyday routine life. A special aspect of the study is the gender focus on men. This area was chosen for several reasons: firstly, to narrow the circle of research for its better detail and quality, secondly, a similar study is being prepared by another postgraduate student of Prof. Kryvosheia and highlights the feminine aspect. Thus, our works will complement each other and explain this problem in detail.

Since the dominant majority of the nobility of Kyiv Province were of Polish origin, this led to the formation of chronological boundaries that cover the period 1793–1917, namely from the liquidation of the Polish-Lithuanian Commonwealth by its third division to the revolutionary events in the Russian Empire, which led to the liquidation of the nobility in the territory of Right-Bank Ukraine. That is, from the liquidation of the Polish state to the beginning of its reproduction. The geographical boundaries of the study cover the territory of Kyiv province in the above-mentioned period.

My scientific work consists of 4 sections, which reveal the issues of education, upbringing, family relations, leisure, and social and economic activities. Thus, the first chapter concentrates on the research and analysis of the source base of the postgraduate work. The second highlights the upbringing and education of men from noble families. The third analyzes family-marital relations and examines the role and place of the husband in the noble family. The fourth is devoted to private and public life. In this way, the study will highlight all key aspects of the daily life of a Polish nobleman in the Kyiv province.

When writing a scientific work, various sources are used: archival materials, the work of other researchers, memories, diaries, correspondence, contemporary press, and others. It is worth highlighting the importance of memories, diaries and correspondence. After all, it is in them that a large part of the

information devoted to everyday life is concentrated. The authors of these sources are direct participants in the events of that time. Therefore, when working with these sources, one should understand their emotional colour and try to critically analyze them. Also, source materials and periodicals of that period are important sources for research. They help to clarify and supplement other materials.

Interdisciplinarity is an integral part of my research because the methods of other disciplines are used in scientific work to implement the tasks. For example, work is carried out with statistical data that help better describe certain study aspects. Also, the use of memoir literature requires appropriate research methods.

To write this research paper, I need to visit other countries to collect the necessary materials. For example, in January 2022, I had a one-month internship at the University of Warsaw at the Faculty of Arte Liberalis under the NAWA program in Poland. During the internship, I had the pleasure of meeting one of the leading researchers on this issue, prof. Tadeusz Epstein. He was working with materials at the National Warsaw Library, the Library of the University of Warsaw, the Library of the Institute of the History of Poland, and the Archive of Ancient Acts. Based on the results of the collected materials, an article was written, which will soon be published in the Kraków publication "Textus et Studia".

In parallel with writing a scientific paper, I take an active part in various scientific events, both national and international, dedicated to the area of my research: meetings, conferences, round-table discussions, etc.

The process of collecting the necessary material for writing the research is being completed, and several articles related to the work are being prepared in parallel. In the summer, I plan to make several trips to the Kyiv archives and the Vinnytsia and Cherkasy archives. A trip to Warsaw is planned for September, but it is not yet known whether this intention is going to be realized. It is planned to finish writing a research paper based on collected sources within the next two years.