2024 IEEE 14th International Conference "Nanomaterials: Applications & Properties" (NAP – 2024)
Riga, Latvia, September 8-13, 2024

Latvian Academy of Sciences
University of Latvia
Institute of Electronics and Computer Sciences
Sumy State University
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# 2024 IEEE 14th International Conference "Nanomaterials: Applications & Properties" (NAP-2024)

NANOmaterials: Applications & Properties-2024

# BOOK OF ABSTRACTS

*Institute of Electrical and Electronics Engineers*
*2024*

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# Book of Abstracts

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TRACK 1

# “BIOPHOTONICS – RIGA SYMPOSIUM”

# New Directions in Correlative Multimodal Imaging (CMI) – Tattoos Removal as Case Study

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**Abstract ID #BP-0929**

Correlated Multimodal Imaging (CMI) gathers information about exactly the same specimen with two or more complementary modalities that – in combination – create a composite and complementary view of the sample [1]. During our talk we will present an overview of the field of CMI and focus on current efforts to bridge the gap between preclinical and biological imaging. As a case study we will present a new way that extracting and quantifying the optical properties by combining 4 different imaging techniques based on spectral and spatial diffuse reflectance measurements. The developed technique was potentially could be applied in the real-life clinical setting where the popularity of tattoos correlates high causing individuals to seek tattoo removal. People tend to remove tattoos for different reasons, such as career goals, social conditions, religious faith, and personal status. To achieve holistic information on tattoos in the tissue context upon the correlation of the data. It will allow generating a multidimensional data landscape on tattoos to establish ways to remove them. It will further enable the development of detection and monitoring modalities for quantifying, tracing, and tracking the ink in the tattoo in vivo and can be translated to technologies that assess therapeutic success for tattoo removals [2, 3].

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# Proteins Stabilized Fluorescent Gold Nanoclusters for Multimodal Cancer Theragnostics

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**Abstract ID #BP-0932**

Cancer is a leading cause of death, taking away millions of lives worldwide annually and remains a global health challenge, and the main treatment methods lack effectiveness and specificity. As of today, individual diagnostic and therapeutic methods used in clinics to detect early-stage cancer and successful treatment are often insufficient. Cancer remains one of the diseases with a high level of complexity that necessitates multidiagnostic and treatment procedures.

Nanotechnology is one of the most promising current approaches for developing novel diagnostic and treatment methods in accomplishing more personalized medicine. In the last decade, ample efforts were dedicated to the development of molecular and particle agents that can be used for both cancer diagnosis and treatment. The field of such research known as "theragnostics", a term used to characterize the combined therapeutic and diagnostic tasks performed by a single system, has resulted in a more precise cancer diagnosis and therapy. These multimodal theragnostic platforms combine the diagnostics and treatment, and, therefore, can eliminate multi-step medical procedures, reduce delays in treatment, and improve patient-care and early diagnostics.

Moreover, nanomedicine integrates the cancer detection and treatment features in one nanoparticle offers multifunctionality for the simultaneously multimodal detection and treatment of the cancer using theragnostic nanoparticles have the potential to revolutionize effective cancer treatment and early cancer detection.

We demonstrate that protein-stabilized gold nanoclusters (PSNCs) have a wide photoluminescence band in the tissue transparency window, generate reactive oxygen species under irradiation with visible light [1, 2], could be labelled with the radioactive technetium-99m (99mTe) [3] and synthesized directly in patient blood plasma [4].

Patient plasma proteins stabilized gold nanoclusters accumulate in breast cancer cells, are non-toxic in the dark, while appear phototoxic under irradiation with visible light. PSNCs are promising theragnostic systems that can be excited to render both: fluorescence emission for optical biopsy, generation of reactive oxygen species for photodynamic therapy. Labeled with 99mTe PSNCs could be used as a contrast agent and shows promise as potential diagnostic agents for bloodstream imaging of the excretory organs in vivo. The results positively confirm their fluorescent properties, stability, and low toxicity, the utility of patient plasma protein stabilized gold nanoclusters for the use in for personalized multimodal cancer theragnostics.

In summary, for the first time we have demonstrated that patient plasma stabilized and 99mTe labeled PSNCs can behave as a multimodal nanoplatform, presenting at the same time potential as PDT effectors as fluorescent biomarkers and potential diagnostic agents.

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# Diagnosis of Neoplasms in Veterinary Medicine Samples Using Artificial Intelligence

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**Abstract ID #BP-0942**

Cancer remains a significant contributor to morbidity and mortality among companion animals[1], particularly in canines and felines, where neoplasm-related mortality rates soar to 18%, escalating to 45% among those aged over 10 years. Cutaneous neoplasms, constituting up to 30% of all canine neoplasms, encompass mastocytomas 16.8%, soft tissue sarcomas 10.9-25.6%, and benign lipomas 8.5-12.5%[2,3]. Fine-Needle Aspiration Cytology (FNAC) has been a mainstay in diagnosing certain skin tumors in veterinary medicine. However, even with experienced veterinarians, FNAC's sensitivity and specificity in detecting malignant skin and subcutaneous tumors are reported at 68.6% and 77.2%[4], respectively. Thus, there is a need for more accurate diagnostic techniques. In response, we conducted a study of supervised machine learning algorithms for differentiating between canine and feline (sub-)cutaneous cancer types. Utilizing a dataset of 20 lipoma, 20 mastocytoma, and 20 soft tissue sarcoma samples, five linear classifiers were applied to statistically significant morphologic features derived from microscopic images. Results indicate that benign lipomas can be differentiated from malignant mastocytomas with an accuracy of 72.5-82.5%, sensitivity of 65-90%, specificity of 70-100%, and precision of 71.4-100%. Similarly, benign lipomas can be distinguished from malignant sarcomas with an accuracy of 82.5-95%, sensitivity of 80-95%, specificity of 85-100%, and precision of 84.2-100%. Comparatively, some of our machine learning algorithms demonstrates higher specificity and sensitivity than FNAC, suggesting its potential as a smart prediction tool for differential diagnosis in veterinary oncology. Integration with non-invasive diagnostic technologies such as ultrasonic imaging holds promise for further improving diagnostic accuracy and treatment outcomes.

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# In Vivo Assessment of the Influence of Aging on Human Skin Using an Innovative Bimodal Approach

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**Abstract ID #BP-0943**

Our group has recently introduced a methodology for noninvasive assessment of structure and composition of human skin in vivo by combining two optical techniques [1]. First, diffuse reflectance spectra in visible part of the spectrum are measured using a compact integrating sphere with internal light source. The second technique, pulsed photothermal radiometry, involves irradiation with a millisecond light pulse at 532 nm and recording the resulting transient increase of blackbody emission from the skin surface using a fast mid-infrared camera ($\lambda$ = 3–5 μm). Both data are fitted simultaneously with the corresponding predictions of a dedicated Monte Carlo model of light transport and heat diffusion in a four-layer optical model of human skin [1].

The described methodology enables assessment of physiologically relevant properties of skin, e.g., the fractional blood content and oxygen saturation, independently for the papillary and reticular dermis [1, 2]. An augmented version of the described approach was used for monitoring of hemoglobin and bilirubin dynamics in traumatic bruises in human volunteers [3] and provisional estimate of the time of injury. Another adaptation enabled objective characterization of black tattoos in human skin and their response to laser tattoo removal treatment using different irradiation settings [4].

This presentation will focus on our recent analyses of the effects of person's age on the thickness and scattering properties of the epidermis and dermis. Multiple linear regression analysis was applied to remove the strong influences of the individually varying melanin and blood contents on the results obtained from 32 measurements in healthy volunteers (age 23–63 years) [5]. The results indicate a gradual decrease of the reduced scattering coefficient in dermis with person's age, on average by 0.25 mm-1 per decade ($p < 0.0001$), while the epidermal scattering and both thicknesses appear unaffected by aging.

**ACKNOWLEDGMENTS**

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# Recent Biophotonics Projects of Riga Group

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**Abstract ID #BP-0957**

The main projects completed or continued in the Biophotonics Lab of Institute of Atomic Physics and Spectroscopy at University of Latvia over the years 2022 and 2023 will be briefly reviewed. The basic funding sources have been European Regional Development Fund, Latvian Council of Science and tri-late ral Latvia-Lithuania-Taiwan collaboration programme. The topics span from human and animal skin studies to the activity control of micro-organisms. Some of the project titles are listed below:

- Multimodal imaging technology for in-vivo diagnostics of skin malformations;

- Effective identification and multimodal diagnosis system for rare skin diseases;

- Fast and cost-effective machine learning based system for microorganism growth analysis;

- Multimodal imaging for veterinary oncology using a combination of optical coherence tomography and photoacoustic microscopy;

- Dynamic laser speckle imaging for evaluation of fungal growth activity;

- Non-melanoma skin cancer diagnostics by evaluating autofluorescence photobleaching kinetics;

- Highly sensitive whole body spectral imaging device for dermatology;

- Histological recognition and analysis of veterinary tumors surgical margins by using artificial intelligence and multimodal imaging.

More details of the Institute project can be found at https://www.asi.lu.lv/en/.

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Support of European Regional Development Fund and Latvian Council of Science is highly appreciated.

# Introduction about understanding interaction light – biological surfaces: possibility for new electronic materials and devices (PhoBioS)

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**Abstract ID #BP-0976**

Various biological surfaces are known to be covered by elaborated micro- and nano-structures, serving a number of functions (e.g. anti-reflective, structural coloration, anti-fouling, pro- or anti-adhesive, etc.) and inspiring numerous industrial applications. Recent years have witnessed a remarkable boost in research in this field. To a large extent, this boost owes to the increasing interdisciplinary of approaches being applied to the study of structured biosurfaces. Sciences as different as classical zoology and botany are inseminated with the advances in genetics and molecular biology; biologists collaborate more and more with nanotechnologists, materials scientists and engineers – all these contribute to the widening of the horizons of research on micro- and nano-structured biological surfaces, and to biomimetic and bioengineering applications of these surfaces in industry. We aim at 'riding the wave' of these developments with our proposal. In our talk I will present the main goal of the COST Action "Understanding interaction light – biological surfaces: possibility for new electronic materials and devices".

**ACKNOWLEDGMENTS**

Introduction about understanding interaction light – biological surfaces: possibility for new electronic materials and devices (PhoBioS).

European cooperation in Science and Technology (COST) – CA21159 Understanding interaction light - biological surfaces: possibility for new electronic materials and devices

# Spectral and Spatial Characteristics of $TPPS_4$ Aggregates

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**Abstract ID #BP-0988**

Porphyrin compounds are widespread in nature and are of big importance in many biological processes. Molecular self-assembly is a spontaneous process that governs the formation of ordered aggregates and plays a key role in abiogenesis. Naturally derived as well as synthetic porphyrin compounds are extensively studied for biomedical and technical applications such as photodynamic therapy (PDT) or photovoltaic systems.

In particular, 5,10,15,20-Tetrakis(4-sulfonatophenyl) porphyrin ($TPPS_4$) has been widely investigated due to its ability to form noncovalently bound supramolecular structures by self-assembly [1]. The different types of the self-assembling aggregates can be formed by changing the $TPPS_4$ concentration and pH of aqueous environment. Although $TPPS_4$ J-aggregates are very well known, there is a lack of deeper understanding about different aggregate formations dependant on the environmental conditions, especially at the pH = 7 and pH = – 1.

It is well known, that TPPS4 molecules, at right environmental conditions, self-assemble into tubular J-type aggregates (indicated J band at 490 nm), which can be shown via Atomic Force Microscopy imaging. Until now, it was believed that TPPS4 molecules do not aggregate in neutral pH. But our investigation in a broad TPPS4 concentration range, shows that at high concentrations of photosensitizer (above $1\times10^{-3}$M), $TPPS_4$ absorption spectrum undergoes changes that indicate formation of aggregates. Even though Soret band (at 414nm) remains constant, Q1 and Q4 bands shifts to red spectral region while intensity of Q2 and Q3 bands changes significantly. These spectral changes indicate aggregate formation, which are different type (not J-type) and could be considered H-type. At neutral pH TPPS4 molecule has a net charge of -2. When pH is highly acidic (-1), TPPS4 molecule has a net charge of +2 (due to protonation of nitrogen atoms in the porphine ring and $SO_3$- groups). This should prevent it from self-aggregating, but at high concentrations ($c> 1\times10^{-3}$M), TPPS4 molecules begin to form aggregates, which are indicated by bands appearing at 426 nm, 490 nm and 702 nm.

In this study we showed that $TPPS_4$ molecules can form at least several structural types of aggregates, depending on $TPPS_4$ concentration and pH of environment. The principles governing hierarchical self-assembly of $TPPS_4$ aggregates may have played a role at the initial stages of abiogenesis. Similar principles of aggregates formation could be used to design structures for light harvesting in artificial photosynthesis, molecular electronics and design required supramolecular structures. Investigation of self-aggregating photosensitizers also gives more insights to the limitations of their application in photodynamic cancer therapy.

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# Automated Classification of Pollens Relevant to Veterinary Medicine

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**Abstract ID #BP-0997**

Pollen monitoring is helpful for medical purposes, weather or crop forecasting, and climate change analysis. Several automatic pollen sampling and identification systems based on digital microscopy, elastic light scattering, fluorescence, and digital holography have been proposed as an aid for real-time monitoring. Pollens are important aeroallergens also in veterinary medicine, leading to flares of atopic dermatitis in dogs, cutaneous or respiratory allergy in horses, and feline atopic syndrome. In this study, we tested a machine learning model, MobileNet V3 Large, for pollen classification in whole slide images. We included four pollen types relevant to veterinary medicine: Bermuda (Cynodon dactylon) and Timothy grass (Phleum pratense), silver birch (Betula pendula), and olive tree (Olea europaea). The average classification accuracy was 88 %. Most misidentifications occurred between the two grass pollens. After grouping Bermuda and Timothy grass together, the average classification accuracy increased to 98%. We showed that the machine learning model can be beneficial for the automated identification of pollens relevant to veterinary medicine.

# Multifunctional Fluorescence Carbon Nanoparticles Developed from Mmicrobiological Waste for Imaging Cancer Cells, Bacteria, and DNA, Adjuvants for Viruses and Antibiotics, and Metal Sensors

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**Abstract ID #BP-1009**

This study presents a novel approach for synthesizing CNPs from discarded microbiological agar media, a hazardous environmental waste. The process involves a two-step treatment of desalted media with hydrothermal treatment and incineration, followed by purification and functionalization. The synthesized CNPs were characterized using diverse techniques, revealing their structural, optical, and surface functional properties. UV-Vis Spectrophotometry was used to analyze the purified CNPs after membrane filtration. The CNPs were functionalised using bovine serum albumin and also by trehalose sugar. The structural and optical properties of CNPs were studied using SEM-EDX and XRD. Surface functionality, particle size, and surface charge were studied using FTIR and dynamic light scattering, respectively. Notably, the CNPs exhibited a 20% quantum yield, enabling their application in metal ion (Zn, Fe, Ca, Pb, and Mg) detection, particularly lead in petrol, due to efficient quenching capabilities. Additionally, CNPs (1-10µl) demonstrated the potential to replace Ethidium Bromide for DNA and RNA visualization and displayed remarkable antioxidant activity. Furthermore, the biocompatibility of CNPs was evaluated using MTT assay and cell imaging on L-132 lung normal cell line, HeLa immortal cell line, and MCF-7 cancer cells and also bacteria visualization. Interestingly, the CNPs acted as adjuvants to bacteriophage, which inhibit the multi-drug resistance E. coli bacteria and also antibiotics' adjuvants with second-generation cephalosporin and beta-lactam antibiotics to enhance their efficacy against various bacterial strains, i.e. E. coli, S. aureus, and Microbacterium maritypicum. The CNPs also have excellent antioxidant properties. The study also revealed their anti-biofilm potential using 200 ppm CNPs. Thus, fluorescent crystalline CNPs open up new possibilities for their application. This is the first report to develop the fluorescence carbon nanoparticles using discarded microbiological solid media. The work was submitted for the patent.

**ACKNOWLEDGMENTS**

it is indipendent research no finincial support avaibale for research

# Theoretical Analysis of Magnetic Levitation Technique and In Vivo Validation on Oral Cancer Diagnosis

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**Abstract ID #BP-1030**

Biomedical magnetic levitation systems which are the combination magnets and optical observation tools have been applied in directing, clustering, separating, or determining the densities of biological cell structures under the influence of gravitation and magnetic forces. [1-3] The utilization of magnetic levitation systems in cell type determination or viability studies and especially in cancer diagnostics is found to be remarkable, however, to our knowledge, these systems have not yet been managed in oral cancer diagnostic studies. In the present study, the designed magnetic levitation system was assembled with two 3x12x63 mm magnets with the same poles facing each other and an optical observation setup. The distance between the magnets and the paramagnetic ion density as two parameters that can tune the magnetic forces in these systems, were theoretically analyzed [4]. For a linear measurement system, the highest sensitivity was achieved at a spacing of 2 mm between magnets, and paramagnetic ion Gd concentration of 30 mM, taking into account the component of the magnetic forces in the direction of gravity. The results of the theoretical investigation were tested and validated ex-vivo with micro plastic spheres of known density and commercial oral squamous cell carcinoma cell line (OSCC) (CAL-27) and healthy oral keratinocyte Primary Gingival Keratinocyte (PGK) cell line. Thereafter, the densities of oral epithelial cells obtained by brush biopsy from 10 people either with OSCC or benign oral lesions were measured with the prepared system in-vivo. The density of the cells taken from benign and cancerous individuals were measured as 1.050+-0.01 g/cc and 1.065+-0.005 g/cc. The cellular density values of the oral benign and malignant cells were successfully determined in-vivo by the developed magnetic levitation-based density measurement system, indicating that it can be utilized for clinical diagnosis of OSCC.

## ACKNOWLEDGMENTS

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# Multimodal Spectroscopic And Imaging Methodology for Skin Diagnostics

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**Abstract ID #BP-1036**

The rising incidence of skin cancer, in particular melanoma, highlights the need for improved detection. We develop multimodal systems for an optical biopsy as alternative to invasive procedures by combining spectroscopic and imaging techniques, showing the potential for improved diagnostics in future.

**ACKNOWLEDGMENTS**

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# An In-based Metal-organic Framework/Perovskite QD Composite for the Sensitive Optical Detection of Chloramphenicol Antibiotics

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**Abstract ID #BP-1059**

The illegitimate use and disposal of antibiotics has been turned into a threat to the environment and ecosystem. As a result, surveillance of many such antibiotics has been an alarming need to safeguard public health. The different metal-organic frameworks and their composites-based electrochemical sensing platforms have been explored over the decade for the various applications of environmental pollutants such as antibiotics, heavy metals, food toxins, and dyes. This work presents the development of Indium metal-organic framework incorporated fluorescent methylammonium lead halide perovskite quantum dots based sensitive optical detection platform for chloramphenicol antibiotics residues in water. The optical-based sensing platform was designed on a flexible transparent substrate (PET) with the deposition of In-MOF followed by deposition of MAPB QDs by drop casting method. The spectroscopic and morphological characterization of the fabricated composite has been performed on FT-IR, UV-Vis, XRD, XPS, and electron microscopy. The developed In-MOF and MAPB QDs-based sensing platform is found to be optically active as showing fluorescence emission at λem=515 nm when excitation λex=295 nm. In the optimized conditions, the developed sensing platform shows the responsive behavior to the chloramphenicol antibiotics even at a very high linear range of concentrations (0.1-1000 ng/mL) with R2 =0.989. The limit of detection of 0.086 ng/mL and the limit of quantitation of 0.15 ng/mL was attained in a short response time on this optical platform. The selectivity studies with other antibiotics were also studied. As a highlight of this research work, the In-MOF/ MAPB QDs-based detection platform for chloramphenicol antibiotics with improved performance due to fluorescent perovskite QDs. In addition, improved sensitivity has been achieved over many of the previously reported optical sensors.

## ACKNOWLEDGMENTS

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# In Vivo Autofluorescence Photobleaching Imaging of Non-melanoma Skin Cancers

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**Abstract ID #BP-1060**

Non-melanoma skin cancers, also known as keratinocyte carcinomas are the most common group of cancers in the general population with an increasing incidence [1]. Therefore, there is a rising need for new noninvasive diagnostic methods that can simplify medical assessment and reduce the cost associated with the diagnosis and management of treatment of these diseases which often involves multiple visits to different specialists and various tests. The two types of non-melanoma skin cancer are basal cell carcinoma and squamous cell carcinoma, their names denoting the layer of cutaneous cells that are affected.

Autofluorescence imaging and autofluorescence photobleaching imaging are methods that use excitation light to produce autofluorescence from the endogenous fluorophores found in the skin. Studies have shown that skin cancer has changed fluorophore concentration compared to healthy skin due to the altered metabolism of the skin cells [2] which is also detectable using imaging [3]. However, the exact mechanism is not fully understood. By separating the green and red channels of the imaging data and looking at separated photobleaching rates we are hoping to increase the understanding of different parts of the autofluorescence signal in both types of non-melanoma skin cancer. This could pave the way for new diagnostic methods of these cancers at early stages.

A custom device was used for imaging. For autofluorescence induction a set of four LEDs with a peak wavelength of 405 nm was used. A 515 nm long-pass filter was used to filter out the excitation light from the autofluorescence signal. A CMOS sensor with an objective lens was used to capture the images. Raspberry Pi with a 4G module was used to transmit the images to a cloud server for storage. Images were processed using Python. Autofluorescence intensity and autofluorescence photobleaching signals were extracted and analyzed for each type of non-melanoma skin cancer.

## ACKNOWLEDGMENTS

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# Multimodal Optical Spectroscopy and Machine Learning For Human Skin Cancer In Vivo Diagnosis

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**Abstract ID #BP-1094**

Skin cancers are the most common groups of cancers diagnosed worldwide, among which 90% are non-melanoma skin cancers i.e. Basal Cell Carcinoma (BCC) and Squamous Cell Carcinoma (SCC). Surgery is one of the main steps in treating skin cancer thus resulting in scarring or disfigurement with great impact on patients' quality of life. Skin carcinogenesis modulation factors such as epidermis hyperplasia, collagen enzymatic degradation, overactive cell metabolism, cell pleomorphism, neovascularization etc., are known to modify the optical properties of skin tissues. Thus, the development of non-invasive in vivo optical biopsy methods, to help surgeons in the peri-operative delineation of safety margins, is a major health, social and economic issue.

In the present study, a bimodal system of skin tissue fibered spectroscopy, combining Diffuse Reflectance (DRS) and AutoFluorescence (AFS) measurements, was implemented in the frame of a clinical protocol involving 140 patients with skin carcinomas and Actinic Keratosis (AK). The Spectrolive medical device developed [1,2] includes a multiple optic fiber probe with four source-detector separations from 400 to 1000 µm, a broadband light source for DRS in the spectral range [340-785] nm and five bandpass filtered LED sources for sequential acquisitions of AFS under narrow band excitations between 365 and 415 nm. The clinical protocol consisted in (i) the collection of the clinical examination data (Fitzpatrick chart, Merz scaling, margin delineation), (ii) the spectroscopic acquisition methodology (number and position of the measurements), (iii) the skin tissue resection (surgery) and (iv) the histological analysis of all the excised samples used as reference classification. The multidimensional spectroscopic data set collected [3] was analyzed using a Machine Learning-based approach for automatic supervised classification [4]. Several combination strategies of feature extraction methods (principal component analysis, non-negative matrix factorization, autoencoder), classifiers (support vector machine, linear discriminant analysis, multilayer perceptron, random forest) and data or decision fusion methods (stacking, majority voting) were evaluated. Highest values of accuracy between 83% and 87% were obtained for pair-wise classification comparing BCC and/or SCC vs healthy tissues, with optimized hyperparameters of our classification pipeline.

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# Correlation Analysis of Heart Rate Variability Between PPG and ECG Compared with a Smart Photonic Device in Supine, Sitting, and Standimg Postures

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**Abstract ID #BP-1098**

In this study, correlation of heart rate variability (HRV) results in supine, sitting, and standing with ECG-based, mobile Elite HRV app, and reflective photoplethysmographic (PPG) pulse measurement devices are explored. HRVs were analyzed with the means of the Poincaré plots. It is not yet clearly indicated whether HRV can be replaced by PRV which also could reflect changes in autonomic nervous function (ANS) and peripheral arterial elasticity. We synchronize electrocardiogram (ECG) signal for HRV and PPG for PRV at 1 kHz sampling frequency with 16 bit. ECG is the best indicator for the assessment of physical health and heart information [1, 2]. By using Photonic device such as PPG which uses light sensor to detect the change of blood volume in the peripheral vessel contains different information. Reflective PPG measurements are also less susceptible to power line noise and any electromagnetic interference [3]. A wearable smart mobile phone Elite HRV app (with BlueTooth) and a CorSense sensor was chosen in parallel with the lab made reflective PPG device. The lab made ECG amplifier was chosen as the reference ECG device.

Participants were volunteers aged 22–79 years from the city and students at Oulu University, Oulu (Finland) to participate in 25 subjects during the year 2024, provided they did not have cardiac diseases or there were no other criteria for exclusion. The results show that in supine, sitting, and standing position (3x5min), the HRV results of the Elite HRV and the reflective PPG finger sensor are of significant positive correlation with the HRV results of the ECG device. Also between each test the blood pressure was measured. The Variance Inflation Factor (VIF) being over 100 for the young persons, while under 10 for the elderly persons. The VIF is equal to 1/(1-r) and r represents the linear correlation coefficient value. The VIF method is appropriate for validation of the regression model.

The VIF is an integer number >2 (e.g. r=0,5) to 1000 compared to the decimal number (r<1 always), and VIF is easy-to-use. The Elite HRV app is also slightly better in many cases than the reflective PPG prototype. The HRV results of the PPG sensor on the right hand and the CorSense sensor on the left hand also show a significant positive correlation (VIF is under 10 for elderly, but over 100 for young) which could show the feasibility of parallel measurements with the reflective PPG and the CorSense sensor. The measurement performance at the supine position with hands at the same level of the heart is better compared with sitting or standing position as the ECG reference based on the VIF numbers. This is important as the consideration also when testing different aged subjects especially in the cases of elderly persons.

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# Investigation of Lensless On-Chip Microscopy for High-Fidelity Hologram Reconstruction and Visualization of Pollen Samples

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**Abstract ID #BP-1100**

Lensless on-chip microscopy offers a compact and cost-effective approach for acquiring in-line holograms of samples positioned near an imaging sensor. Compared to conventional microscopy, these holograms capture both amplitude and phase information, enabling numerical reconstruction and refocusing of sample images, and determination of sample optical thickness. The high space-bandwidth product of the lensless on-chip microscopy makes it a suitable candidate for monitoring airborne particulate matter, such as allergenic pollen, which impacts human and animal health.

A prerequisite for reliable detection and identification of diverse pollen grains is the acquisition of high-quality holograms and the implementation of robust reconstruction algorithms to suppress the twin-image artifact. On the one hand, we experimentally investigate the influence of key parameters on the acquisition of holograms pertaining to light sources and imaging sensors such as spectral width, central wavelength, physical size, source-to-object and object-to-sensor distance, and pixel size. Based on this evaluation, we propose an optimal and cost-effective lensless on-chip microscopy setup. On the other hand, we evaluate the ability of commonly utilized hologram reconstruction algorithms to suppress twin-image artifact with respect to intensity discretization, sampling, and noise. Hologram reconstruction algorithms are mostly based on the angular spectrum method and discrete Fourier transform, which inherently suffer from the discretization and sampling artifacts. Therefore, evaluation by accurately modeled holograms is essential. To achieve this, we implement a GPU-accelerated numerical solution to the Rayleigh-Sommerfeld diffraction integral, which enables hologram simulation to a desired accuracy. Subsequently, guidelines for appropriate utilization of the reconstruction algorithms are presented.

Finally, we demonstrate the applicability of the lensless on-chip microscopy for detection and classification of pollen grains by a direct comparison of the reconstructed holograms to co-registered brightfield microscopy images acquired by a high-end commercial microscope.

# Monte Carlo Simulations of Light Propagation in Turbid Media and Estimation of Optical Properties by Deep-Learning Aided Regression

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**Abstract ID #BP-1103**

We introduce a comprehensive workflow employing the open-source PyXOpto library for developing deep learning-aided regression models to efficiently estimate optical properties in turbid media. This process consists of four pivotal steps. Initially, a Monte Carlo (MC) simulation model is constructed, selecting the optimal sample geometry – layered, cylindrical, or voxelated. This is complemented by configuring light sources and detectors suitable for various acquisition or imaging techniques, including optical fiber probes, spatial frequency domain imaging, and contactless multispectral/hyperspectral imaging. The choice between isotropic and anisotropic scattering models, along with corresponding scattering phase functions, tailors the simulation to the tissue characteristics. The MC simulations can be further optimized by limiting the simulation domain to a finite spherical volume.

The second step involves defining and sampling the free parameters of the simulation model based on their expected statistical distributions. This modular approach facilitates adaptation to a wide array of measurement setups and sample types.

In the third step, regression models are built and trained to deduce selected optical parameters from measured data such as spatially-resolved or frequency domain reflectance. This step focuses on model validation and ensuring computational efficiency alongside accuracy.

The final step utilizes optical phantoms to calibrate the regression models, aligning simulated data with empirical observations. The optical phantoms should span the full range of optical properties expected in the observed samples. The computed calibration coefficients should ideally exhibit a very small variability across the optical phantoms – typically less than 2%. A larger variability is a strong indicator of systematic discrepancies between the actual measurement configuration and the underlying simulation model.

This workflow not only streamlines the estimation of optical properties but also enhances the accuracy and applicability of the Monte Carlo light propagation models in biomedical optics, providing a robust framework for future research and application.

# Snapshot Hyperspectral Imaging and Artificial Neural Networks Reveals Microcirculatory Blood Oxygen Saturation

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**Abstract ID #BP-1139**

New emerging multispectral snapshot cameras can enable real-time imaging of hemoglobin oxygen saturation ($sO_2$) in skin, a clinical parameter of great value for many vascular diseases [1]. The gold standard for analyzing multispectral data, inverse Monte Carlo (MC) analysis [2], is however extremely computationally demanding and not well-suited for real-time analysis of spatially resolved datasets. Developing fast algorithms or methods for estimating hemoglobin oxygen saturation from snapshot multispectral imaging (MSI) data is also challenging due to the complexity of sensor characteristics [3].

Therefore, we developed and evaluated a technique where a snapshot filter mosaic camera is utilized for imaging skin tissue $sO_2$ and trained on in vivo MSI data with target values from a calibrated point-measuring reference method. MSI data were acquired from the distal arm during a provocation protocol including baseline, occlusion, and reperfusion recordings. ANNs were trained to estimate $sO_2$ with MSI data as input, targeting data from a validated probe-based system [4]. Performance of ANNs with different properties and training datasets were compared.

Our method enables spatially resolved estimation of skin tissue $sO_2$. Results are comparable to those acquired using a Monte Carlo-based approach when relevant training data are used. In vivo results show that inverse MC and ANN give almost identical $sO_2$ values with a mean absolute error of 1.3%. The ANN implementation analyzed a single image in less than 0.1 s.

Training an ANN on in vivo MSI data covering a wide range of target values acquired during an occlusion protocol enable real-time estimation of $sO_2$ maps. Data from the probe-based reference method can be used as target despite differences in sampling depth and measurement position. ANN can replace inverse MC, enabling real-time imaging of the microcirculatory $sO_2$ in skin tissue.

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# Beyond Conventional Diagnostics: Revealing Blood Microstructures Through the Harnessing Optical Anisotropy with Polarized Light

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**Abstract ID #BP-1151**

Innovations in diagnostic imaging have vastly improved early cancer detection. Our study introduces a pioneering 3D Mueller Matrix (MM) imaging technique, combined with digital holography, to analyze the polycrystalline microstructure of dehydrated blood films. This method exploits the distinctive optical anisotropy of blood proteins, which undergo significant structural changes in the early stages of diseases like cancer. By integrating polarization-holographic recording and differential MM methodologies, we can spatially and quantitatively characterize these changes within blood films. Employing this technique, we have achieved over 90% accuracy in differentiating between healthy individuals and prostate cancer patients. This breakthrough offers a non-invasive, reliable alternative to traditional biopsies, enhancing patient outcomes through early diagnostic intervention. The high precision and potential for rapid, real-time analysis could revolutionize current practices in oncology diagnostics, marking a significant leap towards personalized medicine.

**ACKNOWLEDGMENTS**

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# What Could We Learn about Biological Tissue by Probing It with Polarized Light

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**Abstract ID #BP-1152**

An early detection of pre-cancerous changes in biological tissue and quantitative assessment of their dynamics may help to choose an appropriate treatment and would significantly improve the survival rate and quality of life of the patients. This challenging task requires the development of accurate, low-cost, fast and reliable methods for tissue diagnosis. Different optical techniques have already become a part of the medical doctors' toolkit, helping them with a precise diagnosis. We focus our studies on biomedical applications of multi-spectral imaging Mueller polarimetry that proved its high sensitivity to small alterations of tissue due to by pathology evolution and holds promise to become a new optical modality for assessment of tissue pathological status.

The custom-built liquid crystal-based imaging Mueller polarimetric systems operating in a visible wavelength range were used ex vivo for staging of colon cancerous lesions, detection of cervical intraepithelial neoplasia, digital histology, regenerative medicine, etc. The cancerous polyps, conizations of uterine cervix [1], formalin-fixed and fresh brain specimens [2] were measured with the wide-field imaging Mueller polarimetric system in reflection. The maps of depolarization, linear retardance and orientation of the optical axis of linear birefringent medium obtained from the decomposition of measured Muller matrix images revealed an enhanced contrast between the zones of healthy and pathological tissue. The optical anisotropy of biological tissue related to the presence of extra-cellular matrix of collagen or densely packed nerve bundles within healthy zone of tissue is confirmed by the gold standard histology analysis. Tissue malformations erase this optical anisotropy of healthy tissue by destroying its ordered micro-architecture, which, in turn, leads to the increase of contrast between healthy and pathological zones in polarimetric images of tissue. We suggest using these contrasts for tissue optical biopsy as well as for the detection of borders of pathological lesions.

Transmission Mueller microscopy studies of thin sections of gastric tissue biopsies [3], mouse uterine cervix [4] and artificial skin [5] have also revealed polarimetric image contrasts that are not present in the total transmitted intensity images. Thus, "staining" of tissue with polarized light combined with the machine learning algorithms for image segmentation may significantly reduce the time for histology samples preparation and pave the way to the automated digital histology to support the diagnosis given by of a pathologist.

Our theoretical and numerical polarized Monte Carlo studies shed the light on the origins of the observed contrasts. The new concept of partial Mueller polarimetry that facilitate the translation of this polarimetric modality into clinical practice will be also presented and discussed.

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# Laser Sensing Through Scattering Media at UPC-CD6: from Biophotonics to Polarized Lidar

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**Abstract ID #BP-1159**

UPC-CD6 is a research centre in Barcelona doing both basic and applied research with companies in Optical Engineering. Within this talk the main lines of activity at UPC-CD6 in the field of laser sensing through highly scattering media will be introduced.

A first line of activity refers to laser sensing using self-mixing interferometry (SMI). The technique stands as a coherent sensing technique of very low cost, suitable for biophotonics applications [1]. SMI takes advantage of the back reflected beam at a diffusive surface in order to mix it coherently with the wave in the laser cavity, creating a beat in the laser emission which may be captured. Such signal may be amplified to measure the amplitude, distance, or flowmetry/speed (via Doppler effect) of a surface or liquid. A first application will be presented measuring the arterial pulse wave using such a simple interferometer, without contact [2].

The SMI system, in particular, is especially effective for flow measurements, as long as the Fourier Transform in the signal analysis removes most of the noise due to the faint signal. However, it is unable to separate the flow of different fluid layers, as backscattering at different depths spreads the Doppler peak. We propose a confocal setup for the sensor to to vertically section flow in layers every 100mm, and showing the flow follows closely Poiseuille's law [3]. Such a solution has applications, for instance, in extra-corporeal blood flow control and clot detection. A second obstacle was the need to reduce the laser emission to make it compatible with laser safety regulations for a focused IR beam on skin, while keeping a reasonable signal-to-noise ratio. For this, we proposed including a third cavity which could be used to improve the SNR by creating an overlapping, adjustable interference pattern which constructively interferes with the remaining standing waves [4].

A second line of work at CD6 has involved the generation and validation of a simulation code for laser propagation in highly scattering media. The simulation code, based on a MonteCarlo approach, is currently able to take into account different types of media, and also the propagation of polarized light, which has been traditionally used as a tool for improved imaging in turbid media. Such simulations have been validated and parallelized in a simulation code which has been applied to different use cases [5].

Such simulation system was applied, in particular, to the simulation of use cases outside of biophotonics. In particular, light propagation through highly scattering media in the atmosphere (fog, smoke sand, smog…) or underwater (turbidity in coastal areas) has been developed based in our code, in particular for solutions linked to pulsed light, such as time-of-flight lidar or range-gated imaging. Measurements in fog chambers have proven the usefulness of the model in order to predict the behaviour of polarized litht beams and will be presented in the talk [6].

**ACKNOWLEDGMENTS**

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# Spectral and Spatial Characteristics of $TPPS_3$ and $TPPS_4$ Aggregates

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**Abstract ID #BP-1213**

Among the known molecular building blocks, porphyrins constitute a highly attractive class for functional nanomaterials due to their unique photonic and electronic properties, specifically for their potential applications in photodynamic therapy, nonlinear optics, and for investigation of artificial light harvesting systems that mimic natural photosynthetic receptors [1]. An understanding of both the interaction between the adsorbate molecules and the interaction between adsorbates and the surface is a prerequisite to eventually controlling the self-assembly process in supramolecular aggregation [2].

Here we report the formation of supramolecular structures whose size and aggregation pattern are controlled by changing the number of polar sulfonic groups of sulfonatophenyl porphyrin. On the basis of spectroscopic investigations we show that substituted porphyrin molecules the 5,10,15,20-Tetrakis(4-sulfonatophenyl)porphyrin ($TSPP_4$) and it's 5,10,15-tris(4-sulfonatophenyl)-20-phenylporphyrin analog ($TPPS_3$) exhibit the different spectroscopic and spatial characteristics of self-assembly.

Both ($TPPS_4$) and (TPPS3) have the ability to self-assemble and form J-type aggregates. Under acidic aqueous conditions, the diacid species of the TPPS porphyrin forms J-aggregates due to hydrophobic π-π stacking and electrostatic interaction between the anionic sulfonated phenyl group and the cationic core. As a result of aggregation, 490 nm and 709 nm bands are formed in absorption spectrum. Different types of aggregation depend on the pH and concentration of aqueous solution.

$TPPS_3$ and $TPPS_4$ acquire similar spectral and spatial characteristics, however the lack of one $SO_3$- group compared to $TPPS_4$, impacts big differences of aggregation. Our experiments showed, that $TPPS_3$ $pK_3$ is lower than a value $pK_4$ of $TPPS_4$. As a result, $TPPS_3$ change the symmetry from $D_{2h}$ to $D_{4h}$ earlier and the porphyrin ring of molecule becomes protonated (changes net charge of the molecule) and starts to self-assemble into the aggregates earlier and at lower concentrations value. Atomic microscopy, theoretical calculations and spectroscopy, showed that $TPPS_3$ and $TPPS_4$ are forming different aggregates or differently interacting groups of them.

Our findings suggest that replacement of functional groups in mezzo position of porphyrin ring influenced self-aggregation of TPPS and changes of environment pH, TPPS concentration allow design and construct different supramolecular structures adsorbed to surfaces.

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# Neural Network-Based Feature Prediction Using Remote Photoplethysmogram Waveform Analysis

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**Abstract ID #BP-1231**

The continuous prediction of peripheral blood volume pulse waveforms is of great significance for the prevention and treatment of cardiovascular diseases. The origin of pulse waveform is mainly affected by various factors, such as vascular age, lifestile, and ability of vascular disorders [1]. Non-contact measurements of blood volume pulsations in microvascular tissue can be done by remote photoplethysmography (rPPG). Blood waveform analysis allows the assessment of hemodynamic parameters (HP) related to arterial health, e.g. predicting high risk of patients with type II diabetes [2] or risk of mortality in sepsis patients [3].

This work aims to classify subjects into a specific vascular health condition based on a given pulse waveform using network-based machine learning models. For this reason, we trained our models by 9000 waveforms taken from palm's dorsal side of 18 subjects (14 healthy, age 21-54 yrs. and 4 patients affected by septic shock and taking vasopressors, aged 45-81 yrs.). To get variant waveforms, we employed a bilateral thigh supra-systolic occlusion test in healthy subjects to temporarily compromise leg blood supply, potentially altering vascular resistance.

To train our models, we used 5 sets of HP related to incisura and diastolic amplitude and its curvatures (calculated from SPPG 2nd derivative. The HP were grouped in 5 classes of equally spaced intervals. The classification model validation tests showed the following best accuracy taken from five classes: true-positive 98.8% and false-negative 1.2%. The neural network-based approach could be valuable for prediction of vascular health state from blood pulse waveform in cases when the signal is weak and noisy.

## ACKNOWLEDGMENTS

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# Impact of Bilateral Thigh Occlusion on the Remote Photoplethysmography Signal Recorded from the Palm

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**Abstract ID #BP-1239**

Occlusion of limbs, whether partial or complete, arises from various pathological and physiological conditions affecting blood flow and vascular hemodynamics[1]. Factors such as peripheral arterial disease, certain sleeping postures, or prolonged sitting can lead to occlusion. This phenomenon impacts local blood flow and alters systemic hemodynamics, potentially affecting overall vascular health. Therefore, non-invasive assessment of occlusion's impact on central hemodynamics and its local manifestations holds great importance. In our pilot study, we investigated the effects of bilateral thigh occlusion on systemic hemodynamic parameters and their local manifestations using remote photoplethysmography (PPG)[2] signals from the palmar skin. We employed a bilateral thigh supra-systolic occlusion protocol in eighteen healthy subjects to temporarily compromise leg blood supply, potentially altering hemodynamics. Systemic hemodynamic parameters, including heart rate (HR), mean arterial pressure (MAP), and total peripheral resistance (TPR), were recorded beat-by-beat alongside the palmar PPG signal at 540 nm. Changes in the PPG signal were evaluated by analyzing waveform feature points. Our results revealed significant alterations during occlusion and post-occlusive hyperemic periods. Upon initiating occlusion, temporary fluctuations in MAP, HR, and TPR occurred, lasting for 20-30 seconds. Once stabilized, occlusion led to an increase in MAP (6.6%), TPR (8.8%), HR (4.8%), and the PPG waveform parameter RI (12.8%). In the post-occlusive hyperemic period, consistent declines were observed: MAP reduced by 8.6%, TPR by 37.4%, and RI by 24.2%. These findings suggest that bilateral thigh occlusion significantly alters systemic hemodynamics, leading to increased peripheral vascular resistance, as observed in the palmar PPG. Notably, changes in the waveform, particularly its diastolic component, indicate an increased magnitude of the retrograde pulse wave reflecting at the occlusion site [3]. The present findings demonstrate that bilateral thigh occlusion significantly impacts systemic hemodynamics, increasing peripheral vascular resistance. This effect suggests that bilateral supra-systolic occlusion could serve as a valuable model for the physiological manipulation of vascular resistance in laboratory tests. The observed changes in the photoplethysmography (PPG) waveform during different occlusion protocol stages emphasize the importance of the retrograde pulse wave, which is reflected from the occlusion site and contributes to the genesis of the PPG signal. Collectively, this study highlights the potential of remote PPG in assessing arterial occlusion and vascular resistance, which could prove valuable for evaluating various medical conditions. However, the complex relationship between central hemodynamics and local cutaneous microcirculation responses, influencing the PPG signal, requires further research.

## ACKNOWLEDGMENTS

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# Reference Values of Skin Oxygenation Saturation Using Hyperspectral Imaging: a Study on Healthy Volunteers and Optical Phantoms

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**Abstract ID #BP-1278**

Measurement of cutaneous oxygen saturation ($ScO_2$) on lower limbs, next to a chronic wound if there is any, is supposed to be part of a conventional diagnostic procedure of peripheral arterial disease [1]. However, due to a time-consuming method currently available in clinics (based on Clark electrodes), $ScO_2$ is rarely measured [2] and the development of easy-to-use and fast optical methods sustains improvement in chronic wounds diagnostic management. Knowledge on « normal » values obtained by such innovative optical devices is of utmost medical importance for the correct interpretation of clinical results. Luengo et al. [3] carried out the metrological characterization of two successive generations of InSpectra devices, characterized by two different optical probes, i.e. featuring two different distances between excitation and collection optical fibers (15 and 25 mm respectively): they found statistically different ("normal") reference values in a population of 21 healthy volunteers using one device then the other one (all measurements were acquired on the thenar eminence of all volunteers). Mean ScO2 value was 84 % when measured with the InSpectra 325 (25 mm inter-fiber distance) and 78 % when measured with the InSpectra 650 (15mm inter-fiber distance). In the current study perfomed on 32 healthy volunteers (authorization 21-861 by Institutional Review Board IRB00003888, IORG0003254, FWA00005831), we aim at providing normal $ScO_2$ values obtained with a medical device called Tivita (Diaspective company) based on hyperpsectral imaging. Values were acquired on three anatomical sites: chest (close to the clavicle), palm of the hand (thenar eminence), and ankle (inner malleolus). Statistical tests show a dependence of measured values on anatomical sites ($p<0.05$), on gender (for people older than 50 years, $p=0.02$) but not on age ($p>0.05$). In order to investigate $ScO_2$ values dependence on anatomical site, optical phantoms were developed in order to mimick skin optical properties modifications and thickness variations from one anatomical site to the other one. Dermis was mimicked using agarose gels containing human hemoglobin and epidermis was mimicked using intralipids solutions of different concentrations. Epidermis-mimicking layer thickness was made variable in order to mimick epidermis thickness variability of different body sites. Results show that optical properties variation due to intralipids concentration (i.e. scattering coefficient) variation and to thickness variation has a significant impact of $ScO_2$ values for the same hemoglobin concentration in dermis. Such results contribute to our understanding of skin optical properties impact on $ScO_2$ measurements made in clinics.

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# Terahertz Quantum Cascade Laser Imaging of Human Skin Pathologies: Towards Early Detection of Skin Cancer Using Laser Feedback Interferometry

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**Abstract ID #BP-1348**

Early detection of skin pathologies with current clinical diagnostic tools is challenging, particularly when there are no visible colour changes or morphological cues present on the skin. Terahertz (THz) imaging has long held promise for skin cancer detection but has been hampered by the lack of practical technological implementation. In this work, we present a technique for discriminating several skin pathologies using a coherent THz confocal system based on a THz quantum cascade laser emitting at 2.8 THz . High resolution in-vivo THz images with diffraction limited to the order of 100 μm of several different lesion types were acquired and compared against one another using the amplitude and phase values, applying technique of the optical feedback interferometry. Our system successfully separated pathologies using a combination of phase and amplitude information and their respective surface textures. The large scan field (50 × 40 mm) of the system allows macroscopic visualization of several skin lesions in a single frame. Utilizing THz imaging for dermatological assessment of skin lesions offers substantial additional diagnostic value for clinicians. THz images contain information complementary to the information contained in the conventional digital images. Our findings suggest that THz imaging could provide a feasible imaging modality for skin cancer detection that is beyond the visible.

## ACKNOWLEDGMENTS

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# Upconverting Nanoparticles as Novel Labels for Immunohistochemistry

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**Abstract ID #BP-1354**

Photon-upconversion nanoparticles (UCNPs) are a novel class of labeling agents for immunohistochemistry. UCNPs are near-infrared (NIR) absorbing luminescent nanoparticles with an absorption maximum (976 nm) in the NIR optical window of tissue. Unlike conventional fluorophores emitting light with lower energy/longer wavelength upon excitation, UCNPs absorb more than one photon per excitation process and emit photons with higher energy (shorter wavelength). The NIR excitation and large anti-Stokes shift completely remove tissue autofluorescence, greatly enhancing the sensitivity of the system, enabling the detection of individual UCNPs. UCNPs possess extreme photostability and can thus be handled under ambient light and maintain a constant emission over hundreds of scan cycles. In this presentation I will share some of the outstanding properties of UCNP-based IHC labels.

**ACKNOWLEDGMENTS**

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TRACK 2

# “NANOMATERIALS SYNTHESIS & SELF-ASSEMBLY”

# The Role of Water in Self-Assembled Peptides:Contribution to Structure and Properties.

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**Abstract ID #NSS-0934**

Recently, the focus of research has been on biomolecular piezoelectrics with sufficiently high piezoelectric properties and internal compatibility with the biological environment. Piezoelectricity in biological objects was found in several biological materials of different natures [1]. Short peptides like diphenylalanine (H–Phe–Phe–OH, FF) not only display enhanced semiconducting behavior but also showcase a diverse array of beneficial properties such as high Young's moduli, robust photoluminescence, notable piezoelectricity, pyroelectricity, strong electro-optical effects, and optical waveguiding capabilities, among others. [2-3]. A self-assembly process occurs only in the presence of water molecules, serving as the "glue" that binds FF monomers into elongated nanotubes with a precise 1 nm diameter, which subsequently aggregate into rigid hexagonal bundles known as microtubes. After the self-assembly in an aqueous solution, water molecules remain captured inside the nanochannels and form a layered structure. The first layer is a structural (bound) water forming hydrogen bonds with peptide molecules. The second layer consists of "free" molecules that fill the space near the tube's axis. Sometimes a third layer can be found in between the first two layers.

Water molecules inside the nanochannel stabilize their structure and impact their physical properties. It is assumed that there could be a microporous structure with cylindrical holes based on the FF and the net flow of water molecules through the FF channels is possible [4], which is key for many biological processes occurring in the aquatic environment and can stimulate the use of FF for technological applications. for example, to deliver certain molecules

Furthermore, compelling evidence suggests water's significant role in shaping the mechanical properties of FF structures. Its influence extends to other material characteristics like ionic conductivity and electrochemical storage. Water interaction with the peptide backbone structure may be related to the origin of Alzheimer's disease since nanostructured FF peptides have the same structural motif as Aβ amyloid fibrils. Water plays a key role in the formation of crystalline piezoactive films based on FF dipeptide [5].

This work reviews the influence of different types of water on the structure and properties of self-assembled dipeptides.

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# Formation of Antimicrobial Packaging Biopolymer Nanocomposite Materials for Food Storage

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Formed film materials based on biopolymers polylactide (PLA) and polycaprolactone (PCL) by sputtering Ag nanoparticles onto the surface of the polymer matrix. The presence of metallic silver on the surface of the PLA-PCL film was confirmed by the method of wide-angle X-ray scattering. This is indicated by the presence of two low-intensity maxima at 2θm ~ 38° and 44° on the diffractograms of the samples. These maxima correspond to the crystallographic planes of the face-centered cubic lattice of silver, are characterized by indices (111) and (200), respectively, and confirm the presence of metallic silver on the surface of the polylactide-polycaprolactone film. Analysis of microphotographs of nanocomposites showed that upon sputtering of silver nanoparticles on the surface of the PLA-PCL polymer matrix, a layer with a thickness of ~425 nm is formed.

Biopolymer packaging materials PLA and PLA-PCL with Ag nanoparticles, sprayed for 3 and 5 min, demonstrated antimicrobial effects against S. aureus and E. coli.

The inhibitory effect of the PLA-PCL-Ag film on the number of mesophilic aerobic and facultatively anaerobic microorganisms (KMAFAM) on the 7th day of poultry meat storage was revealed. There was a two orders of magnitude reduction in the total number of molds and yeasts, and the number of E. coli bacteria (E. coli) was 9% lower compared to conventional vacuum film and PLA-PCL film. The absence of pathogenic bacteria of the genus Salmonella spp. and Staphylococcus aureus bacteria in chilled poultry meat samples. In wheat bread (7 days) and in pumpkin seeds (30 days), when using all types of packaging material PLA-PCL, PLA-PCL-Ag and ordinary vacuum film, quantitative changes of microorganisms, yeasts and molds were not observed.

Studies of the antimicrobial action of the PLA-PCL-Ag biopolymer packaging material demonstrated the quality and safety of the created films, because the calculated indicators of both the total number of KMAFAM microorganisms, as well as yeast and mold fungi, correspond to the standards of DSTU.

The obtained data allow us to state that the formed biopolymer packaging materials with antimicrobial properties are promising for the creation of packaging materials for food products, which will allow increasing the shelf life of various groups of products, without changing quality and safety indicators.

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# Employing Biogenic Reagents for the Green Synthesis of Plasmonic Au and Ag Nanostructures for SERS-Based Detection

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**Abstract ID #NSS-0948**

Nanostructured metals have been drawing intense research interest due to their diverse applications across multiple scientific domains. In the case of gold (Au) and silver (Ag), the nanostructures of these strongly plasmonic metals display huge potential in catalytic, biomedical, and sensing applications. Synthetic protocols for Au and Ag nanostructures are typically carried out in solution using suitable chemical reagents that serve specific functions in the formation process. However, many of the commonly used reagents are toxic, costly, and difficult to handle. Our study centers on the use of greener alternative reagents for the preparation of Au and Ag nanostructures. Specifically, we explored the use of simple and low-cost biogenic acids as key reagents for our synthesis. This biogenic acid-mediated synthesis approach was rapidly completed at ambient conditions through a simple benchtop experiment, with water as the solvent. Compared to traditional synthetic methods, our procedure is notably greener, simpler, faster, and cheaper. Certain combinations of biogenic acids were found to produce Au and Ag nanostructures with intricate branched morphologies. The numerous SERS-active hot spots (e.g., tips, junctions) that are present in these branched metal nanostructures have enabled their use as SERS substrates for the sensitive detection of toxic rhodamine 6G dye.

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# Water-Induced Crystal-to-Crystal Transformation: Switchable Mechanical and Luminescent Properties

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**Abstract ID #NSS-0952**

The investigation of mechanical properties (soft or rigid) of organic luminescent crystals has become an emerging field in material science [1-4]. Currently, most research in this field focuses on how to construct soft crystals and improve their performance, with few being able to achieve the regulation of mechanical properties, which is crucial for understanding the structure-property relationship and the application of corresponding materials.

In work, we report on a water-induced "soft-to-rigid" regulation based on an alkoxy chain substituted cyanostilbene derivative (DEA) in its crystal system. Specifically, the pristine crystal of DEA exhibits elasticity with yellow fluorescence. Upon water-assisted vapor fuming, water can form multiple hydrogen bonds with DEA molecule and compel the packing structure transformation, and thus a rigid crystal (DEA-w) with orange fluorescence is obtained. The "soft-to-rigid" transition is attributed to the packing transformation from one-dimensional π column to two-dimensional strong hydrogen bond network, which provides stronger resistance to external deformation. In addition, DEA-w crystal undergoes a typical brittle fracture under cutting, offering excellent processability. This study provides an inspired method for in-situ adjustment of mechanical properties of crystal.

## ACKNOWLEDGMENTS

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# Synthesis and Structural Investigation of Exfoliated Graphite-$(SCN)_n$ Composites

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**Abstract ID #NSS-0953**

Graphene and graphene-related materials are characterized by unique properties that make them promising candidates for various applications, including microelectronics, electrochemical capacitors, transparent electrodes, composite materials, and sensors [1]. Despite the potential, the transition of graphene from laboratory research to practical applications has been relatively slow. This is because the development of simple and practical methods for high-quality, large-scale graphene production is still a challenge. In addition, cost-effective methods for surface functionalization of graphene-based materials are also needed to improve the electrocatalytic properties of complex electrochemical devices. As a result, research on the synthesis and application possibilities of graphene and its related materials remains active and ongoing [2–4].

The aim of this study was to synthesize and structurally investigate exfoliated graphite-polythiocyanogen ($EG(SCN)_n$) composites, intended for use in electrochemical sensors. For this purpose, three graphite precursors with grain sizes of <50 μm, ⩾149 – ⩽840 μm, and 2000 μm were intercalated with sulfuric acid and heat-treated at a temperature of 800 °C to acquire exfoliated graphite (EG). The EG samples were further modified with conducting polymer polythiocyanogen ($(SCN)_n$). The obtained $EG(SCN)_n$ samples were characterized using scanning electron microscopy (SEM), Fourier-transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), and Brunauer-Emmett-Teller (BET) analysis.

SEM micrographs revealed the presence of small, rounded particles, confirming the formation of the conducting polymer. FTIR analysis showed the existence of the transmittance bands at about 1246 $cm^{-1}$ (–C–N= stretching vibrations) and 1644 $cm^{-1}$ (=C=N– symmetric and asymmetric stretching vibrations) also confirming that $EG(SCN)_n$ compounds were obtained. XRD analysis showed that all newly obtained samples were characterized by the same interplanar distance (0.334 nm), however, the crystallite size varied. The smallest crystallite size (15.76 nm) was characteristic of sample $EG(SCN)_n$_3, obtained from the largest-size graphite grains. BET analysis revealed that the largest surface area (31.02 $m2 \cdot g^{-1}$) was also characteristic of the sample $EG(SCN)_n$_3. In our upcoming research, we aim to explore the significance of the determined physical properties of synthesized $EG(SCN)_n$ compounds by subjecting them to electrochemical analysis.

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# Fabrication of Polyethersulfone/Reduced Graphene Oxide (rGO) Nanofiltration Membranes for Efficient Removal of $Mg^{2+}$ Ions from Groundwater

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**Abstract ID #NSS-0984**

Magnesium ions ($Mg^{2+}$) are vital components of drinking water, influencing its taste, and health implications. As essential minerals, $Mg^{2+}$ ions play a crucial role in human, contributing to enzyme function, nerve transmission and muscle concentration [1]. The excessive amounts of $Mg^{2+}$ in drinking water can have varying impacts on human health such as gastrointestinal and kidney conditions [2]. The World Health Organization (WHO) provides guidelines to maintain safe levels of $Mg^{2+}$ ions in drinking water, typically recommending concentrations between 25-50 mg/L [1]. Adhering to these guidelines helps ensure that magnesium levels in drinking water remain beneficial without causing adverse health effects, promoting overall well-being for consumers. Nanofiltration (NF) is a highly effective membrane-based filtration technology that holds great promise for the removal of $Mg^{2+}$ from drinking water. NF membranes exhibit size-based exclusion mechanisms that selectively retain $Mg^{2+}$ ions due to their molecular weight [3]. Additionally, NF membranes demonstrate charge-based selectivity through Donnan exclusion, where the negatively charged functional groups on the membrane surface interact strongly with the divalent $Mg^{2+}$ ions, further enhancing their retention [4]. This technology is further supported by the ability of NF membranes to remove $Mg^{2+}$ ion complexes formed with organic matter in water. By optimizing operating parameters such as feedwater pH and pressure, NF membranes can achieve removal efficiencies exceeding 90%, ensuring the delivery of safe and healthy drinking water by effectively mitigating the health risks associated with elevated $Mg^{2+}$ ion levels [5].

In this study, mixed matrix membranes (MMMs) were prepared through phase inversion method. This research aims to fabricate polyethersulfone (PES) nanofiltration membranes impregnated with reduced graphene oxide (rGO) for selective removal of $Mg^{2+}$ ions from groundwater. The physiochemical properties and surface morphologies of the as-synthesized rGO and fabricated membranes were examined using advanced characterization techniques. FTIR spectrum of GO revealed vibration modes corresponding to oxygen-containing functional groups. A broad peak was observed at 3295.8 $cm^{-1}$, which was attributed to O-H stretching mode due to absorbed water molecules. Peaks observed at 1046 $cm^{-1}$, 1200 $cm^{-1}$ and 1500 $cm^{-1}$ are due to stretching vibration modes of C–O bonds and C–OH vibration modes, respectively. The surface morphology of PES-rGO membranes appeared relatively smooth with irregular distribution of rGO sheets, resulting in minimal alterations in pore size distribution and moderate enhancement of hydrophilicity. Furthermore, a notable improvement in $Mg^{2+}$ ions removal efficiency was observed from PES-rGO membranes as compared to the pristine PES membrane. This enhancement is attributed to the additional active sites on the surface of PES-rGO membranes subsequently, enhancing the removal efficiency.

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# Deposition Of Amorphous Molybdenum Silicide (MoSi) Superconducting Thin Films viaMagnetron Co-Sputtering

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**Abstract ID #NSS-1000**

In this work, growth of amorphous superconductive molybdenum silicide (MoSi) thin films on flat and nanostructured substrates was demonstrated. The deposition process involved direct-current (DC) magnetron co-sputtering from molybdenum and silicon targets in argon atmosphere. MoSi films were deposited on oxidized silicon wafers, and $Ga_2O_3$ and ZnS nanowires (NWs). Four-point Cr/Au (3/50 nm) electrical contacts were defined on the thin films and on individual $Ga_2O_3$-MoSi and ZnS-MoSi core-shell NWs using lithography for low-temperature measurements. The molybdenum-to-silicon ratio was optimized to achieve highest critical temperature ($T_c$) of 7.5 K in $Mo_{0.77}Si_{0.23}$. Development of novel superconductive nanostructured materials could enable novel applications in electronics and quantum technologies in future.

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# Investigating Features of Hydrated C60 Fullerenes Obtained by Vacuum-Sublimation Cryogenic Deposition Method: Characterization via Raman, UV-Vis, Mass Spectrometry, and IR Analysis.

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**Abstract ID #NSS-1001**

Fullerenes, a molecular allotropic form of carbon with a spherical geometry, have been extensively investigated for their complex interactions, that resulted in the exploration of fullerene-water molecular-colloidal solutions (FWCS) as detailed in references [1-4]. This complex demonstrates interesing physical and chemical characteristics, encompassing catalytic potential and photoluminescence, with a primary application in biophysics and biology that related to its antioxidant properties [5].

In this study, we introduce a novel approach using the vacuum-sublimation cryogenic deposition (VS-CD) method to produce FWCS. The melting process of the solid phase of the mixture obtained by combined condensation of $C_{60}$ fullerene and water vapors onto a surface cooled with liquid nitrogen results in the formation of a stable colloidal solution. The results of characterization of FWCS via Raman, IR, and UV-Vis spectroscopy with a comparison with literature data on hydrated fullerenes, revealed the presence of $C_{60}$@{$H_2O$}n complexes of hydrated $C_{60}$ fullerene within the solution. Furthermore, transmission electron microscopy revealed predominantly small $C_{60}$ clusters from 2 to 5 nm size within the VS-CD-produced material. Mass spectrometry with laser desorption/ionization further confirmed the existence of pure fullerene $C_{60}$ while ruling out any transformation. Our analysis reveals the close similarity between the stable $C_{60}$@{$H_2O$}n complexes generated by VS-CD and the previously known highly hydrophilic hydrated fullerene obtained by ultrasonication method, highlighting the potential of VS-CD as a promising technique in the synthesis of colloidal fullerene solutions.

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# Growth and Characterization of Weyl Semimetal $WTe_2$ Nanowires

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**Abstract ID #NSS-1048**

Tungsten ditelluride ($WTe_2$), has recently attracted vast interest due to its unique electronic structure leading to intrinsic two-dimensional topological insulator (2DTI) characteristics. $WTe_2$ is also a Type-II Weyl semimetal in bulk crystals, and notable for higher-order topological insulator states enabling exotic, topologically protected charge transport, promising for applications in spintronics [1,2] and for quantum computing [3–5]. Studies of $WTe_2$ through nanostructures, such as nanowires, with their reduced dimensionality and enhanced surface-to-volume ratio, offer a promising platform to harness the intrinsic properties of $WTe_2$. So far the majority of the first experimental evidence of unconventional properties in $WTe_2$ have been demonstrated in bulk and exfoliated materials, while growth protocols of high–quality $WTe_2$ nanowires need to be advanced.

In this study, we synthesized $WTe_2$ nanowires via a two-step chemical vapor deposition (CVD) process, initially obtaining tungsten oxide ($WO_3$) nanowires using either pure $WO_3$ or a $WO_3$:NaCl mixture precursors, which were then converted to $WTe_2$ via tellurization. The nanowires were integrated into nanodevices for charge carrier transport and Hall effect measurements. Despite challenges arising from rapid oxidation of $WTe_2$ nanowires, charge carrier characteristics over a wide temperature range have been collected confirming the high quality of the nanowires.

In conclusion, the advancement in synthesizing $WTe_2$ nanowires presents a promising avenue for future applications exploiting properties of topological surface states.

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# Soft-templated, Mesoporous $Co_3O_4$ Thin Films for Electrocatalysis of the Oxygen Evolution Reaction

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**Abstract ID #NSS-1051**

Electrocatalytic water splitting is a promising approach to produce hydrogen as renewable energy vector to substitute the fossil fuel in order to achieve a $CO_2$-neutral energy system. However, in a practical electrocatalytic water splitting process, considerable overpotentials (η) are required to motivate both hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) at electrodes. As the OER is generally considered as the efficiency-limiting process of water splitting,[1] the exploration of high-performance, cheap and durable electrocatalysts for the OER is essential to make electrocatalytic water splitting economically competitive to already existing hydrogen production technologies (such as the steam reforming process).

In this perspective talk, the focus will be placed on preparation of mesoporous spinel cobalt oxide (meso-$Co_3O_4$) thin films on conductive substrates by the dip-coating and soft-templating approach using an adapted evaporation-induced self-assembly method [2]. The surface and bulk morphology, crystallographic structure, and surface composition of the mesostructured $Co_3O_4$ thin film were correlated to its OER activity. The $Co_3O_4$ nanostructure showed, when applied as an OER catalyst, a low overpotential of 340 mV vs. RHE at 10 mA $cm^{-2}$ in 1 M KOH. The electrochemical performance was evaluated by means of impedance spectroscopy and Tafel plot analysis confirming enhanced electron transfer at the electrode/electrolyte interface. The $Co_3O_4$ electrocatalyst exhibited a promising stability under alkaline conditions over more than 4 hours upon chronopotentiometry (OER-activity loss of only 2% at 10 mA $cm^{-2}$). [3] Also, Ipotential development or optimization approach based on the current system will be mentioned.

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# Ractive RF Induction Plasma Synthesis of Carbon-Encapsulated Nickel Nanoparticles

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**Abstract ID #NSS-1054**

Higher energy density with improved performance of multi-layer ceramic capacitors (MLCCs) has been persistently pursued, achieved by reducing the thickness of the metallic conductive layer, which is accomplished by decreasing nanoparticle size. [1, 2] However, size effects of nanoparticles cause a paradox in MLCC manufacturing as the nickel metallic particle size decreases. A higher surface area to volume ratio makes nanoparticles active, leading to air oxidation and premature sintering, deteriorating the electrical performance of the sintered conductive layer. [3] To solve this paradox, ceramic components are added to the nickel nanoparticles, mainly focused on retarding sintering temperature at the expense of electrical properties. [3] In this context, nickel and carbon binary nanoparticles were chosen to dissolve the MLCC paradox, and Ni/C core/shell structured nanoparticles may be an ideal form for the application. Carbon can be utilized to protect Ni from air oxidation. Ni has a temperature-dependent solubility of carbon in the Ni-C binary system, and therefore, the dissolution-precipitation reaction of C in Ni is used for manipulating sintering temperature and sintered body microstructure. In the present study, Ni-C binary nanoparticles were synthesized by inductively coupled thermal plasma from Ni-C powder feedstock. Characteristics of the synthesized binary nanoparticles were evaluated. Carbon-encapsulated nickel nanoparticles were frequently observed, but strictly speaking, it was a mixture of nickel-rich nanoparticles and carbonaceous nanoparticles. Thick films were prepared by screen printing, binder burn-out, and sintering. Electrical resistance was much reduced compared to pure nickel thick film.

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# Electrochemical Synthesis of AlGaAs/GaAs Nanostructured Heterostructures for Electronic and Optoelectronic Applications

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**Abstract ID #NSS-1057**

This study presents the electrochemical synthesis of AlGaAs/GaAs nanostructured heterostructures and their characterization, elucidating their potential for enhancing electronic and optoelectronic devices. Through an innovative electrochemical deposition process, this research successfully engineered heterostructures exhibiting a unique surface morphology capable of improving light absorption and electronic performance. Notably, due to their tailored electronic and optical properties, the AlGaAs/GaAs interfaces within these heterostructures demonstrate promising applications in LED technology and high-power electronics.

Our findings reveal a granular and plate-like nanostructure morphology characterized by SEM, offering advantageous properties for optoelectronic applications. The composition analysis by EDX further substantiates the material's suitability for such applications. Raman spectroscopy confirms the high crystalline quality and presence of the AlGaAs phase, while PL analysis identifies the distinct optical transitions attributable to the varying Al content in the heterostructures.

The research underscores the methodological advantages of electrochemical synthesis, highlighting its simplicity, cost-effectiveness, and scalability—critical factors for industrial application. The versatility of the synthesis process offers significant flexibility, potentially benefiting a wide range of applications from quantum electronics to cryoelectronics. The study concludes by emphasizing the role of nanostructured AlGaAs/GaAs heterostructures as a cornerstone in advancing innovative electronic materials, paving the way for future innovations in electronics and optoelectronics.

**ACKNOWLEDGMENTS**

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# Charge Transport in High-Quality $WTe_2$ Single Crystals

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**Abstract ID #NSS-1068**

Two-dimensional (2D) materials, including transition metal chalcogenides (TMCs) are promising for a variety of potential applications in electronics, photoelectronics [1], solar cells [2] and other applications. One of the TMCs the most diverse and complex physical properties is tungsten ditelluride $WTe_2$ [3]. It has a large non-saturating magnetoresistance, promising for development of sensors and magnetic memory devices [4]. Due to the low chemical activity of W and Te compounds, growth of high-quality $WTe_2$ is challenging. Ultrathin nanostructures of $WTe_2$ can be fabricated using chemical vapor deposition (CVD) [5], while for applications relying on the large non-saturating, anisotropic magnetoresistance, high-quality single crystals would be needed.

Here we study growth of $WTe_2$ single crystals using the chemical vapor transport (CVT). The CVT approach for $WTe_2$ has been reported in the literature, but more work is needed to understand the charge transport anisotropy, stability of the charge compensation mechanisms, and for practical application in sensor devices.

$WTe_2$ single crystals were grown by the chloride mediated CVT method, using highly reactive $WCl_6$ as a transport agent. The mixture of the W, Te and $WCl_6$ powder was evacuated in quartz ampoule. The ampoule with precursors was then placed horizontally in a two-zone tube furnace. The reaction zone temperature was 900°C and the temperature in the growth zone was set to 700°C for 2-5 days. After the synthesis, the "high temperature end" of the ampoule wall had almost no residual starting material, while the "low temperature end" was covered with ribbon – like crystals in length reaching ~1 cm. The composition was studied using X-ray diffraction analysis, confirming orthorhombic $WTe_2$, in good agreement with JCPDS map number 00-024-1352. Anisotropic charge transport characteristics of the fabricated $WTe_2$ single crystals were studied over a wide range of temperatures from 300 to 2K, using magnetotransport measurements (PPMS Dynacool9T).

**ACKNOWLEDGMENTS**

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# Highly Porous Iron-Nitrogen Co-Doped Graphene Oxide as Excellent Oxygen Reduction Catalyst

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**Abstract ID #NSS-1074**

The first goal of this paper is to report an innovative low-time consuming synthetic method to prepare highly porous iron-nitrogen co-doped graphene oxide (Fe-N/rGO) as few-layer graphene nanosheets, by taking into account that the reduced graphene oxide is one of the most important and available derivatives of graphene, featuring good conductivity and a large specific surface area. Different reaction conditions were considered to produce a series of graphene composites with various nitrogen/iron doping contents (the highest values were N: 9 wt% and Fe: 5%) under microwave field. The resulting materials indicated highly porous and hierarchical structures appearing as sheet-like morphologies. Important challenge still remains in controlling the porosity of the catalyst and distribution of the active sites. The second goal of this paper is to demonstrate that these materials can facilitate oxygen reduction reaction (ORR) in acidic and/or alkaline environments. The electrochemical characterization indicated that Fe-N/rGO – based electrodes could serve as the state-of-art cathode materials, especially in low-temperature fuel cells.

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# Influence of a Magnetic Field on the Luminescence of Highly-dispersed Powder of ZnS:Mn

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**Abstract ID #NSS-1075**

The work carried out studies of highly dispersed powder ZnS:Mn obtained by the method of self-propagating high-temperature synthesis [1]. The concentration of Mn impurity in the samples under investigation was 1 wt%. Sulfur and zinc were taken for synthesis in the ratio close to stoichiometric. The spectra of photoluminescence were measured at a temperature of 1.6 K, the magnetic field changed from 0 T to 5 T. Electronic microscopic studies of ZnS:Mn, and were carried out using scanning electron microscopy (SEM) according to the data obtained, the average particle size of fine ZnS:Mn was ~50 nm. The influence of a magnetic field on the redistribution of the intensity of photoluminescence bands of ZnS:Mn is shown. With an increase in the magnetic field induction, a significant decrease in the intensity of the band caused by the manganese impurity occurs. In this case, the intensity of the self-activated luminescence band does not change significantly

## ACKNOWLEDGMENTS

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# PLA-based and Carbon Nanotubes Modified Materials for 3D Printing

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**Abstract ID #NSS-1077**

Polymer composites filled with nano-sized particles are a wide class of materials with wide application in various fields. Their unique properties arise due to the combination of a plastic polymer matrix and an inorganic nanofiller that has specific characteristics. Recently, the number of studies devoted to polymer nanocomposites containing carbon nanotubes (CNTs) has increased due to the prospect of using such materials as structural and electroactive materials, as well as filaments for 3D printing. However, the ability of CNTs to form aggregates impairs the functional characteristics of polymer nanocomposites and limits their use. Therefore, the purpose of this work is the production of nanocomposite materials using modified CNTs, which have a reduced ability to aggregate. The use of such nanofillers will ensure their uniform distribution in the polymer matrix and contribute to increasing the functional properties of materials for 3D printing.

Polylactic acid (PLA), which is widely used for printing, was chosen as a matrix for creating materials for 3D printing. Functional (electrophysical, thermal and mechanical) properties of nanocomposite materials were studied using electrical impedance spectroscopy, differential scanning calorimetry and stress-strain methods.

Here we show the novel approach for creation of new polymeric nanocomposite materials based on polylactic acid and study of their electrophysical, thermal and mechanical properties. The main idea is the preliminary non-covalent functionalization of CNTs with polyethylene glycol. Such a modification provides a lower aggregation ability and better spatial distribution of nanotubes compared to unmodified CNTs. We have found that modified CNTs significantly affect the functional properties of the polymer matrix at relatively low concentrations of the nanofiller (~ 1%). At the same time, the electrical conductivity, melting and glassing temperatures and mechanical strength exhibit extreme behavior with increasing filler content in the system. It was determined that the greatest effect on the functional properties of the studied systems is observed at a concentration of modified CNTs equal to 1%. It is assumed that in systems based on PLA, there are two mechanisms of the effect of the filler on the polymer matrix: the reinforcing effect of nanofillers, which strengthen and improve the properties of the matrix, and the aggregation of the filler when its amount in the system increases.

We have studied the features of electrophysical, thermal and mechanical properties of new materials with improved functional characteristics. This approach allows us to develop new nanocomposite materials, based on various polymer matrices and functionalized CNTs. The investigated materials with improved properties in the future can be used as filaments for 3D printing and other construction materials.

# Formation and Confinement of Nanoparticles in a DC Glow Discharge

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**Abstract ID #NSS-1092**

This research is devoted to studying the conditions for the formation and retention of nanoparticles in DC glow discharge in acetylene. The discharge tube with an internal diameter of 80 mm was located horizontally. The cathode and anode were flat, with a diameter of 79 mm, and were located vertically within the tube. The distance between them was 76.5 mm. A glass slide for optical microscopes was placed at the bottom of the tube, onto which nanoparticles were deposited. For the subsequent analysis of the deposited nanoparticles using a transmission electron microscope (TEM), separate TEM support grids were located both in the lower part of the tube and its upper part. A voltage of up to 1500 V was applied to the cathode. The experiments were carried out in the range of acetylene flow rates up to 5 sccm and pressures from 0.05 to 0.5 Torr. To visualize the sites of retention and behavior of nanoparticles, a flat light sheet was used, which was formed by splitting a laser beam using a cylindrical lens. The nanoparticle cloud cross-section by the light sheet was recorded using a digital camera.

It has been shown that at a relatively high acetylene pressure (0.15 Torr and higher), a cloud of nanoparticles is formed in the negative glow of the discharge. This cloud usually has the shape of a petal, the dimensions of which depend on the discharge current and gas pressure. Before this cloud appears, a polymer film and small nanoparticles with a diameter of up to 10-20 nm settle on the walls of the tube (both on its upper and lower parts). After the cloud is formed, larger particles of various sizes and shapes fall on the TEM grid. Spherical nanoparticles with a diameter of 100-200 nm or less are usually visible, however, there are conglomerates consisting of many small nanoparticles stuck together in chains. When the discharge burns for a long time, the cathode surface is completely covered with a dielectric polymer film, arc spots run across the cathode surface, piercing the film, and the discharge ceases to be stable. Consequently, the cloud of nanoparticles formed earlier scatters falling to the bottom of the tube and to the anode.

It is well known that nanoparticles in the plasma volume acquire a negative charge. In the glow discharge, negatively charged particles are repelled from the cathode and are expected to move towards the anode. However, in the negative glow, a small potential well may appear that traps negatively charged particles. Nanoparticles can be retained in this potential well for a long time gradually increasing their size due to the attachment of new C2H monomers to them, as well as sticking to each other and forming conglomerates. It is almost impossible to detect such a small potential well using a Langmuir probe while nanoparticles formed in plasma can do this. Therefore, nanoparticles retained in a gas discharge are a valuable diagnostic tool for visualizing the fine structure of the plasma potential distribution.

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# Plasma Polymer Nanoparticles Produced by a Gas Aggregation Source: Challenges Related to their Re-Bouncing from a Substrate

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**Abstract ID #NSS-1122**

Plasma polymers, i.e. macromolecular solids formed as a result of a passage of molecular fragments or precursors through a plasma, represent a highly important class of materials with a broad range of applications. Although these materials are traditionally prepared in the form of thin and ultra-thin homogeneous and conformal films, e.g. by magnetron sputtering, plasma-assisted vacuum thermal decomposition or plasma-enhanced chemical vapor deposition, recent studies proved that plasma polymer nanoparticles (ppNPs) may be also produced. One possible strategy for an effective synthesis of ppNPs is the use of gas aggregation sources (GAS), in which ppNPs formation is due to the spontaneous gas-phase nucleation of plasma-produced molecular fragments or radicals in a high-pressure (tens/hundreds of Pa) aggregation chamber. Such formed ppNPs are subsequently transported by a carrier gas through a small exit orifice from the aggregation zone to the main high-vacuum deposition chamber, where ppNPs are collected [1].

As shown in this study, this approach is applicable to the production of various types of ppNPs (e.g. hydrocarbon (C:H), fluorocarbon (C:F), or oxygen- and nitrogen-containing ones (C:H:N:O)) with tailor-made physicochemical properties (size, chemical composition, etc.). However, unlike the deposition of plasma polymer thin films, a new phenomenon must be accounted for: possible re-bouncing of ppNPs from a substrate to be coated that may result in little or even no deposition rate even though the nanoparticle beam leaving the aggregation chamber is very intense. This effect relates to the relatively high speed of ppNPs (~ 100 m/s) as well as to their mechanical properties. This study aims to demonstrate that two possible strategies may be adopted to promote the sticking of ppNPs on a substrate and thus limit their undesirable reflections that hamper the applicability of GAS systems. The first one is based on an adjustment of their speed before they reach the substrate. As demonstrated by means of the originally developed mechanical velocity filter [2], the speed of ppNPs may be decreased by one order of magnitude by an increase in the pressure in the deposition chamber that substantially reduces their reflection from a substrate. The second possible approach studied in this work is based on the use of a proper substrate. As shown, the complete reflection of ppNPs is limited using nanostructured substrates (e.g., fiber fabrics). In this case, the ppNPs undergo multiple reflections: during each collision with a substrate, ppNPs lose some portion of kinetic energy until they finally land on some fiber. These results are of high importance as they pave the way for the practical use of linker- and solvent-free GAS systems for the deposition of ppNPs.

## ACKNOWLEDGMENTS

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# Highly Tunable Ag Seed Mediated Synthesis and Characterisation of Ag-Au Alloy Nanoparticles Through Controlled Au Growth

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**Abstract ID #NSS-1129**

Alloy nanoparticles containing a homogenous mixture of Ag and Au are increasingly sought after due their enhanced plasmonic and catalytic properties. Synthesis of these alloys is made challenging due to the difference in reduction potential between Ag and Au, which results in the galvanic replacement of Ag with Au. Co-reduction of Ag and Au in varying compositions is one of the more popular means of synthesising alloys but often this results in a lack in control of nanoparticle size and morphology. Seed-based approaches have the opportunity to overcome these limitations but also come with their own challenges and require robust experimental methods in order to create nanoparticles of desired morphology.

In our work, we explore the use of the surfactant CTAC and HEPES buffer to create two separate novel approaches for the directed growth and subsequent homogenisation of Au onto AgNP seeds of around 10 nm. The Au growth proceeds at room temperature, allowing for in-situ spectroscopic monitorisation and mechanistic insights to be elucidated. Alloy homogenisation can be achieved using relatively low temperatures (70°C) within a few hours and allows for tunability of the LSPR across different ratios of Ag-Au. Our work aims to develop a greater understanding of the factors involved in controlling Au growth to make the synthesis of Ag-Au nanoparticles of defined size and composition more accessible to be used for a wide range of applications. In particular, we are also exploring the use of these alloys for plasmon-enhanced photocatalysis in combination with flavins, natural visible light photosensitisers.

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# Influence of $Fe_3O_4$ Nanoparticles on Oxidative Processes and Photosynthetic Pigments of Brassica Napus L., Under Drought.

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**Abstract ID #NSS-1136**

Iron oxide nanoparticles ($Fe_3O_4$) are an important class of nanomaterials that have several unique properties. In this work, we investigated the effect of $Fe_3O_4$ nanoparticles in different concentrations (0, 50, and 100 mg/L) on oxidative processes and production of chlorophyll a, chlorophyll b, and carotenoids under drought as well as adaptation/recovery capabilities in rape Brassica napus L.

The nanoparticles were synthesized using the co-precipitation (Massart) method. For detection of oxidative process in plant the electrochemical measurements of hydrogen peroxide by Co3O4 Nanostructured Electrode were used. The concentration s of chlorophylls (Chl a, Chl b), and total carotenoids were determined spectrophotometrically in acetone extracts of fresh plant material.

Our results show that $Fe_3O_4$ nanoparticles at a concentration of 100 mg/L have a stimulating effect on the production of chlorophylls in rapeseed leaves, but a slight decrease in the production of carotenoids, which indicates their positive effect on the processes of photosynthesis in cell chloroplasts. However, a slight addition of $Fe_3O_4$ nanoparticles to the soil at 50 mg/L did not have a pronounced effect on the plant, and was observed a slight decrease in chlorophyll a and chlorophyll b, which could be caused by the natural processes of plant aging. These results highlight the potential application of $Fe_3O_4$ nanoparticles in agriculture to potentially increase yields and improve product quality by stimulating photochemical processes in plants.

# Fabrication of Carbon Nanostructured Electrodes via CVD Growth on Micromolded Scaffolds

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**Abstract ID #NSS-1141**

Electrode geometry plays an important role in electrochemical processes. Tailoring the electrode morphology by designing and realising complex structures ranging from micro to macro scales can improve mass transport, enhance electrochemical performance and meet the requirements of a particular application. However, reconciling different scale lengths and atomic structures in the realisation of carbon-based electrodes is challenging. In addition, conventional synthesis methods don't provide the flexibility to fully control the electrode mesostructure formation. Here, we present a novel synthesis method that allows control of heterostructure morphology from the macroscale, through the mesoscale, down to the nanoscale by coupling additive manufacturing, phase inversion and microwave plasma enhanced chemical vapour deposition (MPECVD) techniques. In addition, the interfacial molecular structure of the heterostructure (e.g. sp2-C/sp3-C, heterodoping, termination) can be tuned by simply controlling the gas composition and process parameters during the PECVD process. The realisation of topologically optimised heterostructures, characterised by controlled pore structure and chemical composition, paves the way for the development of a fundamental understanding of how architecture determines electrochemical performance and selectivity.

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# Rational Design of AgNPs Reinforced Layered Titanium Phosphate Nanocomposites for Antibacterial Applications

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**Abstract ID #NSS-1142**

The application of titanium phosphate (TiP) materials in the antibacterial area has received considerable attention in the recent few years. This interest stems from their ability to their unique properties: high thermal and chemical stability, corrosion resistance, low toxicity, biocompatibility, formability, and selectivity to target ions and molecules. These properties of TiP surfaces play a decisive role in the biological integration process for their immediate loading and long-term success for antibacterial applications.

The aim of this work was obtained layered titanium phosphate (α-TiP) as supports for "green" synthesized silver nanoparticles (AgNPs) for antibacterial applications. The α-TiP solids were prepared via the sol-gel method followed by microwave-assistaned hydrothermal treatment using the reaction between a titanium isopropoxide and a fosforic acid ($H_3PO_4$). Structural and microscopic studies, using X-ray diffraction, transmittance (TEM), and scanning (SEM) electron microscopies data confirm the resultant plates of a-phases and their enrichment with an average particle size around 100 nm. We showed that the overall preparation process of α-TiP sample having ion-exchange parameters can be seen as a simple and fast way.

The affinity of the α-TiP nanoparticles toward antibacterial agents such as AgNPs was studied in the static conditions. Previously, the series of AgNPs solutions was bioprepared using Melissa extracts and silver(I) acetate solution with various concentrations. The variables affecting the synthesis of AgNPs, including precursor concentration, reducing extract concentration, temperature, and reaction time, were investigated. TEM images demonstrated that obtained AgNPs were spherical shape with the average size from 10 to 15 nm. Since, the antibacterial activity of 12 nm AgNPs was excellent against both Gram-positive and Gram-negative bacteria including Staphylococcus aureus, and Escherichia coli. The as-synthesized AgNPs were incorporated into the α-TiP nanoplates. The successful formation of the α–TiP/AgNPs nanocomposites were confirmed by various techniques TEM images of α–TiP/AgNPs nanocomposites indicate uniform distribution of monodisperse AgNPs without changes in the starting size. Also, IR spectroscopy and thermal gravimetry analysis indicated the significant contribution of polyphenol extract components into the chemical composition of α–TiP/AgNPs. Finally, the antibacterial potential of the α–TiP/AgNPs nanocomposites were evaluated by performing susceptibility tests and time-kill kinetic assays and showed an enhanced antibacterial effect compared to initial nanoformations such as bioactive extract, α–TiP, and AgNPs. The results of antibacterial tests proved that the functionalization of α–TiP/AgNPs nanocomposites provides excellent bactericidal properties against some of the most common pathogens. Thus, the proposed material is simple and minimizes the toxic impact and stability of AgNPs.

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# Synthesis and Characterization of Complex Oxide Phase Nanopowders with a Perovskite Type Structure

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**Abstract ID #NSS-1163**

Today, it is important to create new materials with high magnetic properties. Chemical compounds of iron oxide $Fe_2O_3$ with oxides of rare earth metals $Ln_2O_3$ have special magnetic (ferromagnetic) properties that combine high magnetization and semiconductor or dielectric properties, thanks to which they have been widely used as magnetic materials in radio engineering, radio electronics, computer technology, catalysis, gas separation fuel cells, magneto-optical devices. In recent years, rare-earth orthoferrites $RFeO_3$ have become the research focus for developing multiferroics. Some $RFeO_3$ orthoferrites can exhibit an unusual coexistence of ferroelectricity and weak ferromagnetism [1].

The nanocomposites were obtained by the Pechini method and the heterogeneous precipitation method. Solutions of $La^{3+}$ nitrates, which were obtained by dissolving lanthanum oxides with a content of the main component of 99.99% in nitric acid, were used as starting materials. Before preparing the initial solutions, lanthanum oxide was pre-dried in a muffle at 300 °C for 2 hours. A mixture with different $Fe^{3+}$ content was prepared from nitrate solutions. The obtained precursor was dried at 120 °C for 24 hours and then subjected to heat treatment at 800 °C. Determination of the characteristics of the samples was carried out using physicochemical methods: X-ray diffraction (XRF), thermogravimetric (TG) and differential thermal (DTA) analysis, electron microscopy, and infrared spectroscopy (IR). The samples were subjected to X-ray powder diffraction using a DRON-3 diffractometer at room temperature (Cu-Ka radiation). The scan angle was 0.05–0.1 ° in the range 2q = 15–80 °. The nanocomposites are identified as a perovskite type structure. The XRD patterns do not show any other peaks corresponding to La, $La_2O_3$, $Fe_2O_3$, or any other additional phases associated with impurities. According to SEM, the synthesized powders have a conglomerate structure. According to IR spectra, the synthesized powders have a perovskite type structure. The magnetic properties of the obtained materials were studied.

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# Ferrocene-Enhanced Growth of Millimeters Carbon Nanotube Forests

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**Abstract ID #NSS-1181**

Carbon nanotubes (CNTs) have exhibited outstanding mechanical and functional properties both theoretically and experimentally since their discovery. However, despite their immense potential, their applications remain somewhat limited in certain domains even after three decades of development. This limitation is attributed to various factors, with the small size of CNTs making them challenging to manipulate and explore fully for their intrinsic properties. Growing longer CNTs has thus become a key objective in the field, and while some promising results have been reported in recent years [1-2], challenges persist.

The synthesis of millimeter and centimeter-long carbon nanotubes using the Chemical Vapor Deposition (CVD) method has shown promise. However, the quantities obtained are often insufficient, and the growth rates are too slow for practical industrial production. Identifying the factors limiting growth and proposing innovative solutions to enhance CNT growth rates and extend the lifespan of catalyst nanoparticles are crucial objectives.

In this study, we present recent findings on the role of ferrocene in boosting CVD CNT growth. A conventional CVD reactor was employed, with iron nanoparticles and acetylene serving as catalyst and carbon sources, respectively. Ferrocene was introduced into the reactor through a side-line carrying gas, with its quantity controlled by the gas flow rate and temperature. Remarkably, introducing a small quantity of ferrocene led to a nearly tenfold improvement in the CNT growth rate. This enhancement is attributed to the increased catalytic activity of iron nanoparticles under CVD conditions.

A significant effort was dedicated to evaluating the evolution of catalyst nanoparticles during carbon nanotube growth and their interaction with introduced ferrocene. In-situ gas-atmospheric analyses, along with microscopic studies of CNTs, nanoparticles, and substrates, shed light on the importance of ferrocene under the studied conditions. These findings offer valuable insights for designing more efficient CVD reactors and developing cost-effective procedures that enable the growth of longer CNTs. This research represents a crucial step forward in unlocking the full potential of carbon nanotubes for various industrial applications.

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# Curing Kinetics of Cyanate Ester Resin in Situ N-Phenylaminopropyl Polyhedral Oligomeric Silsesquioxane Nanoparticles

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**Abstract ID #NSS-1190**

Polycyanurates from cyanate ester resins (CER) represent a family of high-performance polymers and exhibit high thermal stability (> 400 °C), high glass transition temperature (> 270 °C), high fire-, radiation and chemical resistance, low water absorption and low outgassing, high adhesion to different substrates and excellent dielectric properties [1]. Due to these attractive features, CER are very promising as highly effective adhesives, sealants, and polymer matrices for composite materials. Improvement of mechanical properties of CER network is successfully reached by adding nanoparticles, especially reactive towards CER.

The present research is focused on investigation of curing kinetics of dicyanate ester of bisphenol E (DCBE) in situ of 10 wt.% N-phenylaminopropyl POSS (NPAP-POSS) possessing eight secondary amino groups active towards the cyanate groups of DCBE. Using FTIR spectroscopy, the conversion of cyanate groups of DCBE was determined at heating from 20 to 300 °C at a heating rate of 0.5 °C/min. Significant differences in the kinetic patterns of the polymerization of the individual DCBE and that in the DCBE/NPAP-POSS mixture were revealed. Thus, in contrast to DCBE, in the DCBE/NPAP-POSS composition, after mixing the components at T=15-20 ° C, a significant increase in the conversion ( α ) of -O-C≡N groups (up to α ≈18%) was unexpectedly recorded. We suggest that at low temperature, the cyanate groups of DCBE mainly react with the amino groups of NPAP-POSS that subsequently leads to the chemical incorporation of NPAP-POSS nanoparticles into the CER network [1]. With further heating of the samples to T=150 °C, the conversion of cyanate groups increases slightly (up to α ≈26%), however, in the temperature range T=160-220 ° C, the reaction rate increases sharply and the main process of polycyclotrimerization of DCBE mainly occurs reaching α ≈ 98% at T=220 ° C. Thus, the NPAP-POSS nanoparticles accelerate the polymerization of DCBE and significantly reduce the final curing temperature.

## ACKNOWLEDGMENTS

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# Facile Sythesis of Band Gap-Tunable Kappa-Carrageenan-Mediated C,S-Doped $TiO_2$ Nanoparticles for Enhanced dye Degradation

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**Abstract ID #NSS-1206**

Recent advancements in semiconductor technology have significantly influenced the field of photocatalysis, particularly for environmental remediation applications [1-3]. This study explores the synthesis of titanium dioxide nanoparticles ($TiO_2$ NPs) using kappa-carrageenan (κ-carrageenan), a naturally occurring polysaccharide, which serves not only as a reducing and stabilizing agent but also as a dopant in the production process. The modified synthesis approach involves the incorporation of sulfate-rich κ-carrageenan, which induces the doping of sulfur and the retention of carbon residues within the $TiO_2$ structure. Comprehensive analysis through Fourier-transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), and energy-dispersive X-ray (EDX) spectroscopy confirms the presence of these dopants. The dual doping significantly alters the electronic properties of the nanoparticles, reducing their band gap to 2.71 eV. This alteration enhances the photocatalytic efficiency of the $TiO_2$ nanoparticles, as demonstrated by their ability to degrade methylene blue and methyl orange dyes by 99.97% and 97.84%, respectively. The results highlight the potential of using κ-carrageenan in the synthesis of $TiO_2$ NPs, presenting an eco-friendly, cost-effective, and highly efficient method for the remediation of harmful organic pollutants. This approach not only advances the field of photocatalysis but also contributes to the development of sustainable technologies for environmental protection.

## ACKNOWLEDGMENTS

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# Enhanced Detection of Histamine in Food Products Using Colorimetric PEGylated Gold Nanoparticles

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**Abstract ID #NSS-1207**

The presence of histamine, a biogenic amine formed during the microbial decarboxylation of amino acids, is a critical concern for food safety and human health [1-3]. This study describes the one-step synthesis of PEGylated gold nanoparticles (PEG-AuNPs) as a novel approach for the rapid, simple, and cost-effective colorimetric detection of histamine in various food products. The synthesized PEG-AuNPs display a surface plasmon resonance (SPR) within the 520–530 nm range and maintain a hydrodynamic size distribution of 20–40 nm. Fourier transform infrared (FT-IR) spectra confirm the successful reduction and stabilization of the gold nanoparticles, with significant peaks indicating the presence of polyethylene glycol (PEG) as a capping agent. Upon interaction with histamine, the PEG-AuNPs exhibit nanoparticle aggregation, as documented by transmission electron microscopy (TEM), along with a notable red shift and a reduction in the absorbance of the SPR peak. This interaction also prompts the emergence of an additional absorption peak at approximately 690 nm. Increasing the concentration of PEG enhances the colloidal stability of the nanoparticles by forming a protective barrier, which effectively impedes aggregation triggered by histamine addition. The developed colorimetric assay allows for the visual detection of histamine at concentrations as low as 30 ppm, with a linear dynamic response from 20 to 100 ppm and a detection limit of 9.357 μM. Notably, the assay exhibits exceptional selectivity for histamine, demonstrating its potential for effective monitoring and enhancing food safety protocols.

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# Photocatalytic Activity of Carrageenan-Mediated Zinc Oxide Nanoparticles for Water Treatment Applications

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**Abstract ID #NSS-1208**

The quest for efficient water treatment technologies has led to the exploration of green synthesis routes for metal oxide nanoparticles, particularly focusing on enhancing their photocatalytic performance [1-3]. In this study, carrageenan extracted from alkali-treated Kappaphycus striatus, commonly known as Katunay itum, was utilized to synthesize zinc oxide nanoparticles using zinc sulfate as the zinc precursor. This innovative approach leveraged the natural residues of carbon and sulfur in carrageenan, which served as non-metal dopants to enhance the photocatalytic properties of the resulting zinc oxide nanoparticles (car-ZnO NPs). Comprehensive physicochemical characterization of these nanoparticles confirmed the successful incorporation of dopants, which significantly influenced their morphological, optical, and chemical properties. Photocatalytic tests revealed that car-ZnO NPs exhibited remarkable efficiencies in degrading methylene blue (MB), methyl orange (MO), and hexavalent chromium, achieving removal rates of 99.41%, 86.22%, and 90.55% respectively, under 120 minutes of irradiation. These rates outperformed those of undoped zinc oxide nanoparticles by 1.38, 1.65, and 1.21 times respectively. The superior performance of car-ZnO NPs was attributed to the effective suppression of photoinduced electron-hole pair recombination and enhanced redox capacity through Z-scheme spatial charge transfer mechanisms. This study not only highlights the potential of carrageenan as a sustainable resource for producing high-efficiency photocatalysts but also advances the application of green synthesized metal oxides in environmental remediation.

## ACKNOWLEDGMENTS

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# Effect of Film Thickness on the Structural, Morphological, Optical, and Electrical Properties of $TiO_2$ Films Prepared Using Sol-Gel Process

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**Abstract ID #NSS-1222**

Due to its intriguing physical, optical, and electrical properties, $TiO_2$ has garnered significant attention for exploration in various application areas. It has been utilized as a photocatalyst, gas sensor, in medical applications, solar cells, space applications, and in electronics and optoelectronic devices, with the recent addition of its use for proton beam monitoring [1]. $TiO_2$ is a wide bandgap semiconductor that naturally exists in several phases, with anatase (tetragonal), rutile (tetragonal), and brookite (orthorhombic) being the most notable phases. The other two phases of $TiO_2$ are metastable and convert to the rutile phase at higher temperatures [2]. Several methods are employed for its preparation, including sol-gel, spray pyrolysis, sputtering, thermal oxidation, chemical vapor deposition (CVD), pulsed laser deposition (PLD), and so on [3]. However, we have opted for the simple, cost-efficient, and robust sol-gel technique for thin film preparation. In our work, we have developed $TiO_2$ thin films of varying thicknesses on 1cm x 1cm quartz substrate using the sol-gel method and annealed all the films at 1000°C temperature. The structural characteristics and phase determination of the films were conducted using X-ray diffraction (XRD). In the XRD analysis, we observed a mixed phase of anatase and rutile for smaller-thickness films, while a dominant rutile phase was observed for higher-thickness films. The morphological investigation was done using scanning electron microscopy (SEM), from which we observed an increase in grain size with the increase in thickness. Moreover, the optical study of the films was done using UV-Visible spectroscopy. The absorption spectra indicated an increase in absorption in the UV region (250-350 nm) with the increase in film thickness. The optical bandgap was measured from the UV-Visible spectroscopy data by performing Tauc plotting, revealing a decrease in the optical bandgap from ~3.1 eV to ~2.8 eV as we moved from lower-thickness to higher-thickness films. Additionally, we conducted electrical characterization to estimate resistance, leakage current, and variation in resistivity with increasing film thickness. For this, we deposited a Titanium/Gold (Ti/Au) contact on top of the films to measure IV characteristics and resistivity. In future work, we aim to study the electrical characteristics of the device by illuminating it with various radiation sources such as UV-source, pulsed laser, and others. The data collected from the experiment will provide insights into how the electrical characteristics of the device change when it is illuminated by a radiation source. The conclusion of our research is to delve deeper into the properties of $TiO_2$ and to improve or optimize existing application processes while also exploring its applications in new fields.

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# Ageing Processes in Functional Ceramics and Thick-Film Elements

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**Abstract ID #NSS-1233**

The degradation kinetics are modeled at the examples of thermally-induced aging effects in the temperature-sensitive spinel-type bulk functional ceramics based on mixed transition-metal manganites and their thick-film structures. It was shown that degradation transformations in these materials, described by an ideal exponential function, are determined exceptionally by one value of activation energy whichever the structural dispersivity of the system. In contrast, the non-exponential degradation kinetics corresponds strongly to two boundary cases, described by stretched (with power index $0<k<1$) or suppressed (with power index $k>1$) exponential-power-low relaxation functions. Both cases can be well simulated using an original PC program, developed based on a general degradation equation presented in a power-like form in dependence on degradation duration and control parameters.

The stretched exponential-power-low character is proper to own degradation transformations in bulk functional ceramics independently on their phase composition and impurities. This type of ageing kinetics was considered at the example of of $Cu_{0.1}Ni_{0.1}Co_{1.6}Mn_{1.2}O_4$ ceramics caused by more than 500-hours annealing at 443 K. The degradation transformations are described by suppressed exponential-power-low kinetics. This type of kinetics was exemplified by a thermally-induced negative change in electrical resistance of $Cu_{0.1}Ni_{0.1}Co_{1.6}Mn_{1.2}O_4$ thick-films. It was established that suppressed character is explained by two interconnected processes, the first one being the burning-off in organic binder remainders and the second one – the penetration of contact material into thick films.

The kinetics dependences of thermally-induced drift of electrical resistance in single-and multilayered temperature-sensitive thick-film structures based on mixed manganices $Cu_{0.1}Ni_{0.1}Co_{1.6}Mn_{1.2}O_4$ (with p+-types of electrical conductivity), $Cu_{0.1}Ni_{0.8}Co_{0.2}Mn_{1.9}O_4$ (with p-types) are investigated also. It is established, that two interconnected processes are activated during degradation test in p- and p+-type thick film - the burning-out of remainders of organic binder between contacting spinel grains with simultaneous Ag penetration into appeared free-volume space. The degradation kinetics are described by the suppressed relaxation function for p- and p+-type thick films and the extended function for p+-p thick-film structures.

# Effect of Photocatalytic Nanoparticles on Structure, Thermomechanical, and Hydrophilic Properties of UV-irradiated PVA–PEG Hydrogels

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**Abstract ID #NSS-1238**

Crosslinking of polymeric hydrogels allows their use as bandages effective for biomedical applications. Electron radiation and freeze-thawing are among the most common methods for crosslinking of polymeric PVA–PEG matrix. The freeze-thawing method is a promising alternative for electron radiation due to its lower cost and scalability. However, freeze-thawing results in hydrogels with reduced hydrophilicity and lower temperatures at which significant changes in mechanical properties occur.

In this study, we demonstrate that incorporating photocatalytic nanoparticles, such as ZnO, $TiO_2$, and Ag, can enhance the crosslinking of the polymer matrix in UV-irradiated, freeze-thawed PVA-PEG hydrogels. Our results show that the operating temperature of freeze-thawed hydrogels increases with the duration of freezing, from 45 to 75 degrees Celsius, while hydrophilicity decreases from 100% to 80%. Ultraviolet irradiation of freeze-thawed hydrogels additionally increases the operating temperature by up to 10 degrees, with photocatalyst-filled hydrogels experiencing a greater increase than non-filled ones. Structural studies indicate that the presence of nanoparticles during UV irradiation enhances crosslinking of hydrogels. The formation and type of cross-linking polymer bonds rely on the method of cross-linking and influence the properties of the hydrogels. Consequently, UV radiation may offer a more accessible method to produce hydrogels with functional properties comparable to those of electron-irradiated hydrogels. By simplifying the cross-linking process, UV radiation could facilitate application of hydrogels across various biomedical fields.

# Self-Organized Nanopatterning of Crystalline Surfaces Induced by Ion Irradiation – Numerical Modelling and in-situ Observation

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**Abstract ID #NSS-1244**

Low-energy ion irradiation of solid surfaces often leads to the formation of self-organized topographical surface patterns on the nanometer scale [1]. Particularly intricate patterns can form on the surface of crystalline Ge(001) at elevated temperatures which enable dynamic recrystallization. It has become clear that a number of different erosive, ballistic, and diffusive effects act simultaneously, and which effects are dominant depends on the surface temperature, ion incidence angle, ion mass, and energy. To elucidate the interplay of these contributions we compare nanoscale patterns produced by irradiation of the crystalline Ge(001) surface with corresponding calculated surface topographies.

In the first study [2], we observed how the pyramidal nanostructures characteristic for the Ge(001) surface are modified when irradiating at off-normal incidence and different azimuthal ion beam directions. For a theoretical description, we propose an anisotropic continuum equation containing both the established diffusive terms and an additional term describing angle-dependent sputter erosion. The main morphological changes resulting from irradiation at off-normal incidence can be reproduced by changing only the coefficients for angle-dependent sputter erosion, which shows the importance of this mechanism for ion-induced nanopattern formation on crystalline surfaces.

In the second study [3], we investigated the morphologies of the Ge(001) surface that are produced by irradiation at normal ion incidence for varying sample temperature, ion energy and flux. Two previously observed kinds of topographies are observed, i.e., patterns consisting of rectangular pyramids and patterns of shallow, isotropic basins. In addition, we find an unexpected third type of pattern for intermediate process parameters, in which characteristic features of the other morphologies are combined. To account for these results, we extended the initial theory to include the effects of the slope and curvature dependence of the sputter yield, showing that the role of erosion is more than the provision of mobile species as previously thought, since it also contributes directly to the actual pattern morphology.

Complementary to these ex-situ investigations, we observed the pattern formation on Ge(001) in-situ by means of grazing incidence small angle x-ray scattering (GISAXS) [4]. Analysis of the GISAXS intensity maps yields the temporal development of geometric parameters characterizing the changing surface morphology from planar to patterned. We compare the observed patterning dynamics in terms of roughening, coarsening, and slope selection with theoretical predictions and adapt our model based on a continuum equation accordingly.

While applications of ion-beam patterned surfaces in bottom-up nanofabrication are already being explored, our work demonstrates that there are still fundamental aspects to be clarified and shows possible routes for gaining these insights.

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# Improved Photocatalytic Water Oxidation of $TiO_2$-based Core-Shell Nanoparticles Using Magnetic Field

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**Abstract ID #NSS-1264**

The present pioneering research study delves into the forefront of nanomaterials science innovations unveiling novel architectural $TiO_2$-based core-shell heterostructures emphasizing the synergistic coupled components for investigation of magnetic field-assisted solar-light-driven photocatalytic water oxidation. Recent reports show the contribution of the magnetic state on the catalytic and photocatalytic response of ferro [1] and ferrimagnetic materials [2]. Moreover, it has been recently shown how the spin polarization of the active catalyst surface controls and enhances the photocatalytic response in Ti-defected $TiO_2$, favoring parallel spin alignment of oxygen atoms during the reaction [3]. This discovery opens opportunities for implementing magnetic enhancement by developing precise engineering of the photocatalyst ($TiO_2$ but also metal oxide/$TiO_2$ combinations). The main aim of the present study consists in the development of multifunctional core-shell nanoheterostructures based on the synergistic combination of lamellar Ferrihydrite uniformly distributed over $TiO_2$ surface, to generate innovative titania-based nanocomposites with enhanced visible light response that can be tested in photocatalytic water oxidation processes to acquire of fundamental knowledge around heterogeneous photocatalysis under magnetic field.

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# Microwave-Assisted Synthesis of $Cu_3N$ and $Cu_3PdN$ Nanocrystals and Their Electrocatalytic Properties

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**Abstract ID #NSS-1279**

ransition metal nitrides (TMNs) represent a class of compounds that remains incompletely explored; nevertheless, their popularity is burgeoning due to their diverse properties and applications. Copper nitride ($Cu_3N$) is a defect-tolerant semiconductor with a cubic anti-$ReO_3$ crystal structure mainly studied for optoelectronics and energy conversion and storage [1]. The vacant space within the unit cell facilitates the intercalation of an additional metal atom into the Cu3N structure. There are numerous reports on the synthesis of ternary copper nitrides; however, they are predominantly confined to advanced physical deposition techniques, such as magnetron sputtering [2].

In this study, a novel microwave-assisted procedure for the synthesis of colloidal $Cu_3N$ and $Cu_3PdN$ nanocrystals (NCs) was developed. Oleylamine was used as both the reducing and capping agent. The size, shape, and surface composition of the NCs were controlled by the reaction time and temperature. In the typical synthesis procedure, $Cu_3N$ and $Cu_3PdN$ NCs of the uniform size of 18 and 11 nm, respectively, were obtained, and characterized by STEM/EDS, HR-TEM, FT-IR, XRD, and XPS techniques. $Cu_3N$ and $Cu_3PdN$ NCs were tested toward their electrocatalytic activity in carbon dioxide reduction reaction ($CO_2RR$), oxygen reduction reaction (ORR), nitrate ($NO_3RR$), and nitrite reduction reactions ($NO_2RR$) by cyclic voltammetry (CV) in a phosphate buffer medium.

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# MXenes: Two-Dimensional, Nano, Quantum, and Scalable

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**Abstract ID #NSS-1286**

MXenes are a family of two-dimensional (2D) early transition metal carbides, nitrides, oxycarbides, carbonitrides, and related structures with a general formula of $M_{n+1}X_nT_x$ , where M is a transition metal, X is carbon or nitrogen (oxygen substitution is possible), T represents the surface terminations (O, OH, halogen, chalcogen, etc.), and n = 1-4 [1]. More than 50 MXene compositions have already been reported, but the number of possible compositions is infinite if one considers solid solutions and combinations of surface terminations. MXenes open an era of computationally driven atomistic design of 2D materials. MXenes possess electronic, optical, mechanical, and electrochemical properties that differentiate them from other materials. Chemically tunable superconductivity has been demonstrated in Nb- and Mo-based MXenes. Chemically tunable ferromagnetism and antiferromagnetism have been predicted. Highly nonlinear optical properties of MXenes are being explored. Several MXenes have been predicted to act as topological insulators and demonstrate the spin Hall effect at room temperature. Many MXenes are metals but with a tunable density of states at the Fermi level, like semiconductors. Moreover, their properties are tunable by design and can be modulated using an ionotronic approach [2], leading to breakthroughs in the fields ranging from optoelectronics, electromagnetic interference shielding, and communication to energy storage, catalysis, sensing, and healthcare. In several applications, such as electromagnetic interference shielding, MXenes have already outperformed all other materials. In this talk, I'll discuss the synthesis and structure of MXenes, their optoelectronic properties, and the coupling between electrochemical redox processes in MXenes and their optical properties, which can be monitored in situ using spectroelectrochemistry techniques [3].

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# $WS_2$ & $MoS_2$ Nanotubes: From Strengthening of Polymers to Artificial Intelligence

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**Abstract ID #NSS-1290**

Study of the multiwall $WS_2$ nanotubes (NTs) behaviour in numerous applications has been demonstrated that rolling of the molecular layers into co-nanocylinders (nanotubes) induces modifications in their structure and results in unusual mechanical, chemical and electrical properties, which appear not only due to size reduction and quantum confinement, but mainly due to curvature, strain and chirality of the layers, inherent to the tubular structure.

The results were implemented into various devices such as solar cell and photodetectors, electrochemical hydrogen evolution reaction (HER), substrate for hydrogen storage, piezoresistive sensors, anodes for Li- and Na-batteries, fillers for reinforcing polymers and artificial vision system. In the recent studies we succeeded to solve the enigma of $MoS_2$ nanotubes syntheis, which was under investigation during more than two decades, and to report on sustainable, catalyst-free and high-yield synthesis of $MoS_2$ nanotubes 20-120 nm in diameter and up to 25 μm in length. Being semiconductors, both $MoS_2$ and $WS_2$ nanotubes are good candidates for photovoltaics and optoelectronics. Additionally, NTs of $MoS_2$ demostrate stronger exciton emission, they are both 40% lighter and 40% stronger compared to their $WS_2$ analogous and hence more beneficial for optical and composite applications. Here a short introduction to growth mechanism of these nanotubes and their most pronounces performance in different applications will be presented.

# The Biomimetic Design and Dispersed Organization of $Ti_3C_2T_x$ MXene Flakes in Cellulose Nanofibers (CNF) Composite Membranes

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**Abstract ID #NSS-1295**

Controlled organization of $Ti_3C_2T_x$ MXene within polymer networks is crucial for harnessing its full potential as a versatile 2D material in a broad spectrum of applications. Cellulose nanofibers (CNFs) extracted from natural plant sources are biodegradable and characterized by high aspect ratio, which provides a large interface area for interaction with MXene flakes. In this work, we develop $Ti_3C_2T_x$/CNFs composite membranes that ensure a controlled arrangement and distribution of single $Ti_3C_2T_x$ MXene flakes within a cellulose matrix with bright light reflection. Leveraging the unique properties of nanofibers with enhanced mechanical strength ultrathin membranes maintain high optical transparency up to 85 % with a volume fraction of MXene flakes < 1%. Our results not only expand the understanding of $Ti_3C_2T_x$/CNFs composites but also illustrate the potential of high-performance composite materials for advanced material science.

# In-Situ Reflectometry For Control Of Nanoporous Alumina Layer Thickness

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**Abstract ID #NSS-1311**

Contemporary nanotechnology faces a deficiency of cost-effective and readily available techniques for synthesizing ordered nanomaterials with a high surface-to-volume ratio [1]. Nanoporous alumina (NPA) templates present a viable solution for fabricating such materials [2]. The geometric properties of NPA can be precisely controlled by adjusting synthesis parameters, such as anodization time and voltage, even during the anodization process. It is crucial to ascertain the thickness of the NPA layer without inflicting damage on the sample to prevent errors in subsequent applications, such as the deposition of gold or silver nanoparticles.

In this study, we use monocrystalline (001) aluminum substrate for producing nanoporous alumina via anodization in 0.3M oxalic acid at a 40V potential. The layer thickness of the synthesized alumina is optically determined during the process. The sample is exposed to visible light, and the reflected light is collected and analyzed. Reflectance is compared to a mathematical model based on the calculation of electromagnetic wave interaction in multi-layered structures using the transfer-matrix method (TMM) [3]. We have confirmed the suitability of the developed method for the synthesis of NPA with sub-wavelength layer thickness (250 nm and above).

The results were validated using spectroscopic ellipsometry, showing a standard deviation of 1-2 nm within each sample. This method of controlling thickness during anodization eliminates the need for sample sectioning for scanning electron microscopy and is particularly beneficial for the small-scale production of PAAO-based functional optical coatings [4]. Additionally, our thickness control methodology is capable of accurately monitoring PAAO thicknesses exceeding 1 μm [4].

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# Porous Anodic Aluminum Oxide – Metal Nanostructure Multilayers for Optical Sensing

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**Abstract ID #NSS-1317**

Low-cost sensor substrates for chemical detection or biomedical diagnostics are in high demand for applications in accessible healthcare, environmental safety, food production or research organizations. Nanostructured materials combine several properties, that are advantageous for optical sensor readout, including large surface area in a small detection volume and strong interaction with light. Multilayered hybrid coating can simultaneously express multiple physical phenomena, such as photoluminescence (PL) [1], propagating or localized surface plasmon (SP) modes and Fabry–Pérot like resonances [2,3]. Interaction between these modes can enhance certain sensor parameters, such as sensitivity or signal to background ratio. Here we demonstrate optical sensor substrates based on multilayer structures obtained by templated deposition of metals on porous anodic aluminum oxide (PAAO) layers with optical subwavelength thickness.

PAAO with a hexagonal pore arrangement, a center-to-center distance of 100 nm, and a pore diameter of 30 nm was created by anodizing aluminum substrates in a 0.3 M oxalic acid electrolyte at a potential of 40 V. Subsequently, the surface was either coated with a thin (20 nm – 30 nm) gold film via thermal evaporation or decorated with gold nanoparticles (AuNP with 40 nm, 60 nm, and 80 nm in diameter) from a colloidal solution. The multilayer systems, consisting of aluminum, a PAAO layer, and either nanoparticle or nanopore arrays, were tested for bulk refractometric sensing of liquids. Additionally, they were utilized for biosensing by functionalizing the gold surface to detect vascular endothelial growth factor A (VEGFA). The sensing was done using spectral analysis of either normally reflected light or scattered light upon angled illumination from a broad-band source.

For AuNP-type substrates in scattering mode, the signal intensity and refractometric sensitivity could be increased by approximately four times by adjusting the PAAO thickness within the subwavelength range of 250 nm to 600 nm [2]. Substrates with 60 nm diameter particles resulted in highest sensitivity exceeding 200 nm per refractive index unit. For substrates with porous Au film, the optical scattering signal was too weak for practical applications, but in reflection mode sufficient signal change was observed by changing VEGFA concentration in 100 – 1000 pg/mL range. Use of PAAO as templates for sensor substrate synthesis is a lithography free process. Furthermore, the colloidal nanoparticle deposition can be done at ambient conditions which is favorable for scalable production.

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TRACK 3

# “ELECTROCHEMISTRY OF NANOMATERIALS”

# Synthesis of Low Cost Condutive Ink for the Fabrication of Screen Printed Eletrode

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**Abstract ID #EN-0913**

Nowadays, there is a growing interest in portable electrochemical sensor for point of care diagnosis. For electrochemical sensing of biomolecule, normally screen printed electrode is used which is small in size and have high accuracy. Despite recent advantages there is a lot to explore for cheap, high performance conductive ink for screen printed electrode. In this work conductive ink has been synthesized using graphite powder, sodium silicate and PEDOT: PSS. Conductive ink basically consists of conductive material, binder and solvent. Mostly the conductive material with less resistance is expensive. Graphite powder is of low cost and easily available conductive material. Sodium silicate is used as binder which thickens the solution and holds the particles together. The PEDOT: PSS used mainly act as a solvent.

The conductive ink was synthesized by mixing graphite powder, sodium silicate and PEDOT: PSS in proper proportion. The properties of conductive ink like resistivity, surface tension, adhesion were studied. The conductivity observed of the as synthesized ink was 201.38ohm/sq. The conductive ink was further characterized by Scanning electron microscopy, Raman spectroscopy, Fourier transform infrared spectroscopy. Therefore this conductive ink brings exciting possibilities for further using it for screen printing on substrate.

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# Diamond Patterning via Sequential Infiltration Synthesis for Biosensing Applications

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**Abstract ID #EN-0916**

Over the past years, there has been significant progress in the sequential infiltration synthesis (SIS) of inorganic materials within nanostructured block copolymer templates, leading to the production of customizable functional nanomaterials [1]. This research aims to employ sequential infiltration synthesis to build a nanopattern on a diamond surface while assessing its electrical properties concerning biosensing applications.

One important application of Sequential Infiltration Synthesis (SIS) is the regulated incorporation of inorganic materials into templates for self-assembled block copolymers (BCPs) using polystyrene-block-poly(methyl methacrylate) [2], to create a variety of line/space or hole patterns by orienting them parallel or perpendicular to surfaces. This technique has applications in biology, chemistry, materials science, physics, and materials research. Interestingly, although it is widely used on silicon substrates [3], it has not been tested on diamonds. The nanoscale objects are carefully shaped by successive incremental molecular assembly activities. Following surface modification with oxygen plasma cleaning, diamond substrates were subjected to BCP self-assembly. Spin-coated and annealed PS-b-PMMA block copolymer films were used to create self-assembled patterns. The SIS method [1], combined with oxidizing agents and metal-organic precursors, produced organic/inorganic hybrid compounds. Before being exposed to the metal precursor vapor, BCPs on diamond diffused into films, preferentially interacting with PMMA domains. The polymeric species were eliminated by plasma etching, revealing a metal oxide nanostructure that resembled the BCP template. Surface graphitic electrodes were created by implantation of 50 keV energy and subsequent annealing strategically located at the surface for precise alignment with nanopatterned diamond surfaces.

The electrochemical properties of both nanopatterned and non-patterned surfaces were analyzed using cyclic voltammetry and amperometric measurements, allowing for a direct comparison of sensitivity and selectivity in biosensing applications.

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# Synthesis, Investigation, and Application of Polypyrrole/Exfoliated Graphite Composites for the Detection of Dopamine

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**Abstract ID #EN-0967**

Graphene and its derivatives are promising candidates for designing rapid and accurate sensors with high sensitivity and selectivity due to their high surface area, chemical stability, and capacity to immobilize a variety of biomolecules [1]. In recent years, due to the important role of dopamine (DA) in the human body, the development of graphene-based electrochemical sensors for its detection has received considerable attention. DA is a catecholamine transmitter and one of the most prominent neurotransmitters of the nervous system, also known as pleasure neurotransmitters [2, 3]. Sufficiently balanced DA is vital for both physical and psychological well-being: DA is responsible for our emotional responses and for the control of muscle movements. Alterations in the optimal concentration of DA are associated with a wide range of ailments such as Parkinson's disease, schizophrenia, hypertension, and heart failure [3]. Thus, the precise determination of DA, as well as the development of sensitive and selective platforms for the detection of DA, has become an important issue in clinical diagnosis, especially at a very low concentration.

The aim of the research was to study and develop electrochemical sensors based on polypyrrole/exfoliated graphite (GPPy) composites for DA detection. For this purpose, three graphite precursors with grain sizes of <50 µm, ⩾149 – ⩽840 µm, and 2000 µm were intercalated with sulfuric acid and heat-treated at a temperature of 800 °C to acquire exfoliated graphite (EG). During the wet-synthesis procedure, EG was further modified with the conductive polymer polypyrrole (PPy) to achieve GPPy samples. The obtained GPPy samples were characterized using scanning electron microscopy (SEM), Fourier-transform infrared spectroscopy (FTIR), X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, and were tested as active electrode materials for the detection of DA.

Raman spectroscopy, FTIR, and XPS confirmed successful nitrogen incorporation into the graphitic structure after PPy modification. In addition, the sample obtained from the medium-size graphite grains (GPPy_2) had the lowest number of defects (ID/IG = 0.483) and the highest elemental nitrogen content (5.12 at.%), with 15.16 % as graphitic-N, known to improve electrocatalytic activity. Electrochemical investigations revealed that the GPPy_2/GCE sensor demonstrated the most promising parameters, including high sensitivity (2180 µA $mM^{-1}$ $cm^{-2}$) and a low limit of the detection value of 78 nM for the DA analyte. The introduction of innovative synthetic modifications offers the prospect of creating advanced materials based on graphene, which could be utilized across a wide range of sectors. This development is expected to positively impact on the advancement of sensing technologies, facilitating improved functionalities and heightened performance capabilities.

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# Study of Core-Shell Metal-Organic Framework Electrodes for High Performance Supercapacitor Applications

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**Abstract ID #EN-0983**

In this investigation, researchers have successfully synthesized a core-shell structure by depositing nanosized ZIF-8 crystals onto the UiO-66 metal organic framework (MOF) using a precise layer-by-layer technique. Contrasted with the pristine UiO-66 and ZIF-8, this core-shell MOF demonstrates a marked enhancement in specific capacitance, representing a significant breakthrough.The heightened performance of the core-shell MOF is ascribed to its exceptional capacity to facilitate swift electrolyte ion diffusion through the nanoscale ZIF-8, thereby augmenting the electron transfer process involving the metal ions within the UiO-66@ZIF-8 architecture. This intricate interplay between the two materials results in a synergistic effect, culminating in superior electrochemical performance.Notably, the core-shell structure achieves an outstanding specific capacitance of 588.8 F/g when evaluated at a current density of 0.5 A/g, utilizing a 1M $H_2SO_4$ aqueous electrolyte. This remarkable outcome underscores the potential of this composite material for advanced energy storage applications, promising significant strides in the field of electrochemical energy storage.

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# Phosphorus-Modified Reduced Graphene Oxide as a Platform for Simultaneous Electrochemical Detection of Dopamine and Uric Acid

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**Abstract ID #EN-0985**

Dopamine (DA) and uric acid (UA) possess close oxidation potentials on traditional electrodes that cause overlapping peaks in electrochemical measurements [1]. Therefore, the electrode modification with graphene-based materials could be a key strategy to improve the selectivity and sensitivity of simultaneous detection of DA and UA [2].

This study aims to synthesize phosphorus-modified reduced graphene oxide (P-rGO) samples and investigate their electrochemical performance in the determination of DA and UA. The P-rGO samples were synthesized by one-pot hydrothermal treatment of GO in the presence of $H_3PO_4$ (10 and 20 wt.%) in a Teflon-lined stainless-steel autoclave at a temperature of 180 °C for 12 hours. Characterization encompassed scanning electron microscopy (SEM), Brunauer-Emmett-Teller (BET) analysis, X-ray photoelectron spectroscopy (XPS), and Raman spectroscopy. Cyclic voltammetry (CV) and differential pulse voltammetry (DPV) measurements were performed to analyze the electrochemical behavior of P-rGO samples toward the detection of DA and UA. XPS confirmed the successful incorporation of P-containing functionalities (such as C-P=O and $PO_x$) within the P-rGO samples. SEM images revealed wrinkled graphene layers in the P-rGO samples, reflecting structural modifications by hydrothermal treatment and incorporation of P-species. The $N_2$ adsorption-desorption curves confirmed the mesoporous nature of the prepared materials. The results of CV and DPV demonstrated well-separated oxidative peaks of DA and UA, confirming a successful simultaneous detection of analytes. The enhanced sensitivity toward the detection of DA and UA was observed with a higher content of P in the P-rGO structure.

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# The Role of Citrate-ions in the Codeposition of Tungsten and Rhenium into Electrolytic Nickel Alloys

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The electrodeposition of binary and ternary tungsten and rhenium alloys (NiW, NiRe, NiWRe) from solutions based on nickel sulfamate in the absence and presence of citrate ions was studied to clarify the role of complexation in the formation process of nickel-refractory metal alloys. It has been shown that NiRe alloys deposited from sulfamate and sulfamate-citrate electrolytes contain 13-55 at.% rhenium, which means the presence of citrate ions in the solution is not a prerequisite for the formation of an electrolytic alloy of this refractory metal with nickel. At the same time, in coatings deposited from a sulfamate electrolyte, the alloy crystal lattice contains nickel perrhenate. Probably, the role of citrate ions in the case of NiRe alloy electrodeposition is to change the mechanism of the process and exclude from it the nickel perrhenate formation stages.

When depositing a NiW alloy from a citrate-free electrolyte, it is possible to form a high-quality coating containing a small amount of tungsten (1.3 at.%) and not containing oxide compounds only with intensive stirring of the solution and removal of "tungsten blue" from the electrode surface. The role of citrate ions in the case of electrodeposition of NiW alloys is not only to bind into complexes the tungstate ion existing in the bulk of the solution, but also to bind tungsten-containing anions of intermediate oxidation states into complex compounds which can be adsorbed and discharged on the electrode and can be not removed from the surface by the resulting convection currents.

Coatings of ternary NiWRe alloy are characterized by a decrease in the content of both refractory metals compared to their binary alloys. When the concentration of citrate ions is half of the total concentration of refractory metal ions, citrate is spent on the formation of complexes with tungstate ion. Despite the fact that citrate ions are released as a result of the reaction and can again participate in complex formation on the surface, they do not take part in the discharge of perrhenate ions, and the electrodeposition of rhenium into the ternary alloy take place the mechanism with the formation of $Ni(ReO_4)_2$.

# Improvement of β-SiC/por-Si/mono-Si Heterostructures for Supercapacitor Applications by Mitigating Lattice Mismatch and Improving Electrochemical Performance

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**Abstract ID #EN-1056**

This research introduces a novel β-SiC/por-Si/mono-Si heterostructure fabrication method aimed at addressing the challenges of lattice mismatch and enhancing electrochemical performance for supercapacitor applications. Integrating a porous silicon buffer layer mitigates strain, enhances adhesion, and reduces defect densities in SiC films. Comprehensive structural and crystalline assessments are conducted using SEM, EDX, XRD, and Raman spectroscopy, revealing an orderly and pure morphology with high crystallinity. Our results indicate significant potential for supercapacitors, evidenced by an increased surface area for charge storage and a stable electrode-electrolyte interface, crucial for rapid energy delivery and high-power applications. The straightforward carbonization process also underscores this technology's scalability and industrial viability. By effectively addressing the issue of packing defects in SiC films, this study advances the application of SiC in high-performance supercapacitors and other semiconductor devices that require high-frequency and high-power capabilities.

**ACKNOWLEDGMENTS**

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# Graphene Oxide – Gold Nanoparticles Hybrids for Enzyme Free H2O2 Detection

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**Abstract ID #EN-1067**

Graphene oxide (GO) and reduced graphene oxides (RGOs) show intrinsics electrocatlytic activity towards the electrocatalytic reduction of H2O2. Combining these materials with gold nanoparticles results in highly sensitive electrodes reaching the sensitivity at the nanomolar range [1],[2] as the electrocatalytic properties of GO and nanoparticles are synergistically enhanced. Among effects influencing the synergy are defects and surface composition of the GO material can be studied by Raman and infrared spectra [3].

In the current contribution we study the hybrid materials composed of gold nanostructures having shapes of nanospheres, nanourchins and nanobowls [4]. All materials were characterized by electron microscopy, infrared and Raman spectra. The interaction between nanoparticles and GO is visualized by the relative intensities of Raman bands (ID/IG) and other parameters in the Raman spectra. The differences in Raman intensities are directly related to the electrocatalytic properties suggesting that defects in the graphene structure are main factor influencing the electrocatalytic properties. In this contribution we systematically discuss the co-relation between the infrared, Raman and electrochemical characteristics on the hybrid electrodes.

## ACKNOWLEDGMENTS

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# Pt-Fe Nanoparticles Supported on Graphene Oxide for Durable Proton Exchange Membrane Fuel Cells

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**Abstract ID #EN-1070**

Proton electrolyte membrane fuel cells (PEMFCs) have demonstrated high energy conversion efficiencies and low environmental pollution for converting hydrogen and oxygen into electricity. In spite of considerable efforts to develop advanced Pt-based catalysts to improve the active area of platinum during the oxygen reduction reaction (ORR), high activities and/or durability are still an inconvenience for technological or commercial transfer of PEMFCs. Here we report a hybrid electrocatalyst (Pt-Fe/rGO) that consists of Pt–Fe nanoparticles supported on reduced graphene oxide support. A low-time consuming and single-step synthesis method for bimetallic catalyst supported on graphene oxide is proposed, starting from commercial graphene oxide, metal precursors and reducing agent. Electrochemical measurements indicated that the presence of Pt-Fe/rGO enhance the electrocatalytic activity and stability for ORR indicating that it is an effective candidate for practical application for PEMFCs. The multiple active sites of prepared catalyst result not only in a higher mass activity for Pt, but also in an excellent durability. The performance loss is negligible even after standard potential cycles, and no current drop was observed at 0.6 V in a fuel cell test with Pt-Fe loading at the cathode. The obtained results indicated the importance of the synergistic effects between Pt-Fe active sites to design more active and durable low-Pt electrocatalysts for fuel cells, and more importantly, the proposed synthesis route represents a solution for the prepation of advanced metal-doped graphene oxide, with various application in catalysis.

## ACKNOWLEDGMENTS

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# Production of Nanosized Carbon Electrodes Using Acetylene Gas for Scanning Electrochemical Microscopy Probe

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**Abstract ID #EN-1071**

Nanoelectrodes have revolutionized electrochemistry by providing insight into the realm of single molecules. Unlike conventional electrodes, which interact with large molecule ensembles, these microscopic tools, with dimensions in the nanometer range, offer unprecedented capabilities such as heightened sensitivity and a high surface-to-volume ratio, enabling the study of molecular-level kinetics. Carbon-deposited nanoelectrodes enhance sensitivity, stability, and electrochemical activity, making them versatile and cost-effective solutions for various sensing, biomedical, and environmental applications.

In this work, we have fabricated carbon nanoelectrodes (CNEs) with a tip diameter of 20–50 nm, working as a tip for SECM. The capillary for the CNEs has been prepared with the laser pulling method, in which a quartz glass capillary is subjected to heat and tension from a laser, resulting in a tapered fine-tip microelectrode core with a tip of 20–50 nm in diameter. Subsequently, a carbon layer is deposited via pyrolysis of acetylene gas using a flame of butane gas producing a temperature of 1300–1500 °C in a controlled environment with argon gas at the glass tip, facilitating carbon deposition in the capillary without interfering with air. The prepared CNE has been characterized with a scanning electron microscope and scanning electrochemical microscopy (SECM) to determine the morphology of carbon at the tip as well as the electrochemical properties of the tip for use as a probe for SECM. When used as a probe for SECM, it showed typical CV behaviour of the microelectrode with a limiting current in the range of 6–20 pA for different sizes of tip diameter. The work done allows us to explore the possibility of using nanoelectrodes to determine surface activity at the nanoscale in various applications such as biological sensors, energy storage and harvesting, and corrosion applications.

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# Seeded Growth of Tungsten Ditelluride Nanostructures

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**Abstract ID #EN-1085**

wo-dimensional transition metal dichalcogenides (TDMs) have captured tremendous scientific interest in various research fields due to their wide range of promising applications in nanoelectronic and optoelectronic devices. A recent discovery of intrinsic 2D topological insulator properties and superconductivity in one of the TMDs – monolayer $WTe_2$ [1,2] has actualised demand for reproducible fabrication of high-quality mono- and few-layer $WTe_2$. Flake exfoliation from bulk crystal and chemical vapour deposition (CVD) are the two common methods. While being more reliable than exfoliation, so far demonstrated CVD growth of mono- and few-layer WTe2 does not provide sufficient control over placement and quality (number of layers, homogeneity) of the fabricated structures. One promising avenue would be to use CVD with pre-defined seeds, well-studied approach for TMDs, but this has not been extended for $WTe_2$ so far.

Here we show that by placing precursor material directly on the substrate, controlled growth of tungsten ditelluride can be achieved. For the fabrication of arrays of mono- and few-layer $WTe_2$ nanostructures, lithographically patterned and functionalised $WO_3$ thin films on $SiO_2$ and monolayer h-BN/$SiO_2$ substrates have been used. By adjusting the $WO_3$ structure size, functionalisation material, and growth conditions, such as growth temperature, $H_2$/Ar ratio and flow, arrays of mono- and few-layer $WTe_2$ nanostructures have been fabricated.

Our results show that seeded CVD growth of tungsten ditelluride is a promising method of controllably obtaining pre-defined arrays of mono- and few-layer nanomaterials, particularly important for further studies of unconventional electronic properties.

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# Newly-Developed Al-based Metallic Glasses and Nanocrystalline Alloys with Enhanced Corrosion Resistance

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**Abstract ID #EN-1113**

The glass forming ability (GFA) is analyzed factor in designing the chemical composition of alloys with an amorphous structure [1]. The low GFA factor is a challenge and has significantly limited the use of metallic glasses based on aluminum [1, 2]. The most popular aluminum-based metallic glasses are Al-TM-RE alloys [1-3]. According to the assumptions described in the literature [1-3], the aluminum content should be in the range of 80÷92 at.%, TM 1÷15 at.% and RE 3÷20% [2]. It is very well known that the unique properties including corrosion resistance of metallic glasses are resulted from the lack of structural defects characteristic for crystalline alloys [4].

The aim of this study was to present newly developed chemical composition of two amorphous and two nanocrystalline Al-Ni-Y-Fe alloys with lower aluminum content and enhanced corrosion resistance. The samples were produced in a form of melt-spun ribbons. Structural studies were carried out using X-ray diffraction (XRD), transmission electron microscopy (TEM) and scanning electron microscopy (SEM). In order to describe the corrosion resistance, potentiodynamic measurements and electrochemical impedance spectroscopy (EIS) tests were carried out in 3.5% NaCl aqueous solution at 25℃. Corrosion products were analyzed by SEM observations with energy dispersive X-ray (EDX) analysis.

## ACKNOWLEDGMENTS

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# The Fusion of Nature and Technology: Bioceramic Coatings for Magnesium Alloy Implants

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**Abstract ID #EN-1146**

The emergence of 'green'sustainable biomaterials marks a new area of surface properties, potentially expanding the horizons of the temporary biomedical industry. Plasma electrolytic oxidation (PEO) stands out as a promising technique to achieve this task, by enhancing the corrosion and structural integrity of implant [1]. Nevertheless, the development of biomimetic implant coatings requires on use of calcium phosphate (CaP) compounds [2]. The application of sodium hexametaphosphate as a phosphorus source has been found to beneficially affect the osteoinductive and corrosion properties [3]. Incorporating organic additives into the PEO process presents a attractive solution for improving the protective and biological properties of the coatings. Furthermore, bio-calcium carbonate (bio-$CaCO_3$) derived from eggshells serves as an ideal substrate for generation Ca-based coatings due to its enhanced bioavailability for organism [2]. Thus, our study aims to create a "green" ceramic-based coating that will provide appropriate structural, chemical, and biocompatible properties.

For plasma electrolytic oxidation (PEO) treatment of Mg-based implants, we developed two electrolyte formulations: P9, containing 5 g/L $(NaPO_3)_6$ and 5 g/L NaOH; and P10, compraising 5g/L $(NaPO_3)_6$, 5 g/L NaOH, and 31 g/L bio-$CaCO_3$ from eggshells. The PEO process was conducted under an impulse current with a fixed voltage in 250V, 300V, and 350V. The samples were analyzed by scanning electron microscopy (SEM) equipped with energy-dispersive X-ray spectroscopy (EDX). The surface wettability was measured by static contact angle (CA) measurements.

The fabricated coatings exhibited porous structures that typical for Ca-based PEO coating. EDX analyses confirmed the presence of eggshell particles on the P10 coatings' surface. The P9 coating contained small and uniformly distributed pores with average sizes 0.15±0.2 μm, 0.14±0.3 μm, and 0.3±0.5 μm respectively to apply voltages (250V, 300V and 350V). Notably, the introducing of bio-$CaCO_3$ particle resulted in increasing of average pore size up to 0.4±0.8 μm (300V) and 0.6±1.6 μm (350V) in P10 group. For P9 sample, we detected the increasing of phosphorus by 12% with the elevation of voltage. In contrast, the integration of eggshells did not influence the P concentration. The Ca content varied from voltage and reach up to 10% at 350V. Notably, that incorporation of bio-$CaCO_3$ resulted in significant decreasing of surface wettability up to 32° with using 300 V regime compare to P9 group (range from 65° to 83°).

The set of results indicates that eggshell particles positively impact surface morphology and wettability that opens new perspective for development of nature-inspired coatings on medical implants. To fully understand the implications of these findings, the subsequent phase of research will evaluate the corrosion resistance of the P10 surfaces, as they show promise for more extensive biological investigations.

## ACKNOWLEDGMENTS

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# Photocatalytic Degradation of Pollutants by 2D Material Based Nanochannels for Water Filtration

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**Abstract ID #EN-1160**

The major polluting aspects of our global fashion industries are the textile wastewater that turn black all our freshwater reservoirs. Nano-filtration through membrane technology is one of the biggest solutions of industrial wastewater treatment but the fouling of membrane is the major limitation of previous work. In this research, a novel PVDF/MoS2-TNT (PMT) nanocomposite membranes were fabricated through modified In-situ polymerisation phase inversion method that has the ability of membrane defouling by their excellent photocatalytic activity. The oxygen containing functional groups which increase the hydrophilic properties were confirmed by the FTIR analysis. X-ray diffraction (XRD) analysis confirmed the β phase of PVDF within developed PVDF/MoS2-TNT membrane. XPS analysis provide evidence about the presence of specific chemical state of titanium nanotube and molybdenum disulphide which is involved in photocatalytic degradation of pollutant molecules present in wastewater to increase the defouling properties of PMT membrane. Scanning electron microscope (SEM) show that our membranes are porous in nature and their pore size decreased with addition of MoS2-TNT filer content due to its excellent compatibility with polymer. The results illustrate that PVDF/MoS2-TNT membranes have excellent hydrophilic activity that increase the pure water flux (68.8 ± 1.8 L/m2 h-1) in comparison to pure PVDF membrane. PVDF/MoS2-TNT membranes exhibit the excellent filtration efficiency (~97%) for textile wastewater. The reusability of PVDF/MoS2-TNT membranes was approximately 94% due to the defouling ability of developed membrane. PVDF/MoS2-TNT nanocomposite membrane shows the excellent photocatalytic degradation of adsorbed dye contaminants due to the presence of MoS2-TNT nanocomposite. The results and outcomes of the research demonstrates that the PMT membranes has an enormous potential in commercial application of textile wastewater treatment.

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# Development of Electrochemical Glucose Sensors Utilizing Gold Nanorods

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**Abstract ID #EN-1192**

Gold nanoparticles (AuNPs) are one of the most widely used nanomaterials due to their unique physical, chemical, electrical, and biological properties. Since the physicochemical properties of AuNPs can be modified by varying their structural dimensions achieved by different synthesis methods, they are a suitable candidate for colorimetric analysis, biosensors design, fabrication of photothermal transducers, and imaging [1-3].

Among AuNPs, gold nanorods (AuNRs) are in high demand due to the tunability and sensitivity of their longitudinal surface plasmon resonance [4, 5]. The anisotropic structure of AuNRs exhibits two surface plasmon bands corresponding to surface electron oscillation on the transverse and longitudinal sides [6].

The main aim of this research was to apply different types of AuNRs in modelling glucose biosensors. To calculate the electroactive surface area of the electrodes modified with AuNRs the electrochemical method of cyclic voltammetry was performed. Electrochemical glucose detection was performed using chronoamperometry. The results of the electrochemical characterization of electrodes were crucial to a more profound understanding of the potential applications of AuNRs.

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# Electrical Conductivity of Hydrothermally Synthesized $MoO_2$ and $MoO_2$ / rGO Composites

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**Abstract ID #EN-1199**

$MoO_2$ is a promising electrode material for hybrid supercapacitors due to its pseudo-capacitive properties. The formation of composites based on $MoO_2$ and car-bon nanomaterial makes it possible to improve its electro-che-mical performance by increasing the electrode / electrolyte inter-face and increasing the surface redox reaction rate. Ultra-fine $MoO_2$ and $MoO_2$/rGO composites were obtained by the hydrothermal route. The composites were obtained by a joint route when the nucleation of metal oxide nanoparticles and the reduction of colloidal graphene oxide occurred in the same pot. The presence of monoclinic $MoO_2$ was observed for all samples. All samples are charac-te-ri-zed by broadening of the (211) and (312) reflexes. The average crystallite size for pure mesoporous $MoO_2$ is 5.2 nm with a pore size distribution in the range of 5-20 nm and a BET specific surface area of 65 m2/g. The crystallite sizes for the $MoO_2$ phase in $MoO_2$/rGO composites with a mass ratio between metal oxide and graphene components of 1:0.5 and 1:1 are 5.6 and 4.4 nm, respectively. An increase in the rGO component leads to an increase in the BET surface area from 234 and 421 m2/g with the presence of both micro- and mesopores. There is a narrowing of the pore distribution range for the oxide component of the $MoO_2$/rGO composite compared to "pure" $MoO_2$, which is the result of filling the interparticle pores with reduced graphene oxide. The electrical conductivity of the obtained materials was studied by impedance spectroscopy in the temperature range of 25-200°C and fitted with a modified Jonscher model. The calculated activation energy of electrical conductivity for $MoO_2$ is 0.146 ± 0.015 eV. The presence of two con-duction mecha-nisms (acti-va-tion energies of about 0.10 ± 0.01 eV and 0.23 ± 0.01 eV) for $MoO_2$/rGO do-minating at dif-ferent temperatures is observed. The electrical conductivity of rGO decreases with in-crea-sing fre-quen-cy, and vice versa for the oxide component. An increase in the tem-pe-ra-tu-re leads to a redistribution of the electrical conductivity values for the metal oxide and rGO components of the composites.

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# Gold Nanostructure Mediated Copper Ion Detection Based on Glucose Oxidase Inhibition

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**Abstract ID #EN-1232**

The monitoring of copper ion ($Cu^{2+}$) and other heavy metal ion concentrations in water and other sources is required due to the toxic nature of the compounds [1]. This observation is not only vital for environmental health but also has profound implications in medicine, where numerous pharmaceuticals function by inhibiting essential enzymes within biological pathways. Electrochemical sensors can be employed to detect these compounds. Enzymatic biosensors based on enzyme inhibition serve as valuable analytical instruments for fast monitoring and detection of various inhibitors. For example, the effects of $Cu^{2+}$ ion inhibition on enzyme activity can be registered facilitating simple and rapid monitoring of toxic ion concentrations [2].

In this study, we utilize a biosensor based on enzyme glucose oxidase to monitor the inhibitory effects of $Cu^{2+}$ ions. Additionally, we explore the use of gold nanostructures in electrochemical biosensor to amplify the signal [3-4]. Our work specifically investigates the effects of $Cu^{2+}$ ions and AuNS on the biosensor's performance and examines how AuNS contribute to the inhibition process of $Cu^{2+}$ ions.

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# Electrodeposition of Functional Silver-Rhenium Coatings

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**Abstract ID #EN-1243**

Silver-based composites and electrolytic alloys hold a special place among thin-film materials. Interest in silver-rhenium electrolytic coatings arises due to the combination of unique electrical and catalytic properties of silver [1-3] with the mechanical properties of rhenium [4-5]. In the developed aqueous dicyanoargentate-perrhenate bath based on the previously proposed borate-phosphate-carbonate (BPC) buffer electrolyte for silver plating (pH 7), silver-white, matte, smooth, and durable deposits of silver-rhenium electrolytic alloys containing 0.15-13.5 wt.% rhenium were obtained.

The study focused mainly on the influence of bath composition, as well as temperature, stirring, and current density on the composition, current efficiency, morphology, adhesion, porosity and microhardness of the electrolytic alloy. A voltammetric analysis of the electroplating process in the silver-rhenium system was conducted, with additional focus on the role of ethanolamines.

Conditions for obtaining functional Ag-Re coatings containing 0.7–1.5 wt.% Re were determined. Such rhenium content can be achieved by electroplating in the mixed kinetics zone, at potentials corresponding to the half-wave current limit area. The working range of current densities for deposition (0.25–0.6 A dm-2) and temperatures (17–30°C) were established. Such alloys may find application in power electronics and energy, particularly in the manufacture of electrical contacts operating over a wide temperature range

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# Electrochemical Formation of Functional Rhenium Alloys Coatings

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**Abstract ID #EN-1245**

Electrolytic rhenium alloys with nickel, cobalt, and iron are promising modern materials possessing a wide range of valuable properties that allow their use even in extreme conditions. Depending on the ratio of metals in the alloy, these materials can serve as anti-corrosion, hard, and wear-resistant coatings; soft magnetic materials for hermetic contacts; magnetic microsensors; in information recording devices; as catalysts; as a cathode for the HER; and in devices where stability of properties at high temperatures is critical, e.g., in the aerospace and nuclear industries.

Intensive study of rhenium alloys electrodeposition began in the 1990s. To date, more 80 articles have been published in journals with impact factors, half of which appeared in the last five years. Of these, 50 articles are dedicated to Re-alloys containing iron-group metals [1-4]. The main focus has been on Ni-Re alloys, although some results have been published on Co-Re alloys, while research on Fe-Re alloys has been limited.

To achieve the main goal of the current study, namely the creation of scientific foundations for the electrochemical technology of functional coatings from Re alloys, the following steps were taken: (i) new stable, non-toxic complex electrolytes for the deposition of Fe-Re alloys were developed; (ii) results from voltammetric studies of electrode processes occurring during co-deposition of Re into the alloy were analyzed; (iii) the dependencies of the chemical composition, current efficiency, morphology, and structure of the surface of the obtained Fe-Re alloys on the synthesis conditions were determined.

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# Studying Dopamine and Polydopamine as Connecting Agents between Magnetite Nanoparticles and Gold Surfaces: the Role of Cyclic Voltammetry

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**Abstract ID #EN-1292**

An intriguing class of nanomaterials that has been thoroughly investigated for the use in various technological applications are magnetic nanoparticles (MNPs). MNPs have found applications in catalytic processes, memory storage, magnetic separation, magnetic labelling and in biomedical fields. [1, 2] To maximize the performance of $Fe_3O_4$ MNPs and to produce versatile MNPs, it is essential to combine the use of an appropriate architecture, with the desired properties, with the extra contribution of coating materials and surface functionalization.

In this work, dopamine-coated $Fe_3O_4$ NPs ($Fe_3O_4$@DA) and polydopamine-coated $Fe_3O_4$ NPs ($Fe_3O_4$@PDA) were prepared and characterized by FTIR spectroscopy and TEM. Then, the coated NPs were investigated for their adhesion ability on a gold surface by AFM. Furthermore, the samples are used as electrodes and characterized by cyclic voltammetry in a phosphate buffered solution. Unexpected results allowed us to propose a relationship between chemical composition and adhesion ability, going over a fascinating topic with manifold, unexplored possibilities.

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# The Resistance of $Sb_2Te_3$-CNT Heterostructures to Oxidation at Different Humidity Levels Using the Electrochemical Impedance Spectroscopy

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**Abstract ID #EN-1321**

Antimony telluride ($Sb_2Te_3$) is a three-dimensional material with unique electronic and optical properties, which makes it promising for use in thermoelectric modules, photovoltaic technologies, batteries, temperature sensors, and microcoolers. Fabrication of flexible $Sb_2Te_3$-CNT heterostructures by synthesis of $Sb_2Te_3$ nanostructures directly on the CNT network is favorable for thermoelectric applications due to the formation of direct electrical and mechanical contact between the heterostructure components, facilitating charge carrier transfer and simultaneously preventing unwanted nanostructures agglomeration while maintaining flexibility and Seebeck coefficient similar to the bulk $Sb_2Te_3$. Electrochemical impedance spectroscopy (EIS) is a powerful tool for monitoring electrochemical processes under the influence of moisture and identifying possible changes in the structure and characteristics of $Sb_2Te_3$ heterostructures with CNTs at different humidity levels. Our study aims to analyze the oxidation inhibition of $Sb_2Te_3$-CNT heterostructures at different humidity levels using EIS to improve their durability in various working environments.

Samples of $Sb_2Te_3$, MWCNT, and $Sb_2Te_3$-MWCNT heterostructures were prepared on glass plates. EIS spectra were recorded at 0.1–10,000 Hz in a controlled environment with varying relative humidity (5%, 35%, and 70%) at 25°C.

The environmental resistance across all samples remains relatively stable amidst varying humidity levels. $Sb_2Te_3$ exhibits the lowest resistance (500 ± 10 kΩ g-1) due to potentially higher water adsorption, whereas MWCNTs demonstrate notably higher resistance attributed to their hydrophobic nature. Formation of $Sb_2Te_3$/CNT heterostructures leads to a tenfold increase in resistance, suggesting altered surface properties and reduced susceptibility to environmental adsorption. The Faradaic resistance of $Sb_2Te_3$ diminishes as humidity increases, indicating accelerated oxidation kinetics influenced by water presence. Conversely, MWCNTs display high Faradaic resistance and low capacitance, likely due to reduced interaction with water molecules. Increased Faradaic resistance for $Sb_2Te_3$/MWCNT heterostructures indicates a decrease in oxidation processes and changes in electrical characteristics.

The Stern-Geary relationship is employed to assess the inhibition degree of $Sb_2Te_3$ oxidation by MWCNTs. Results reveal significant inhibition, particularly at higher humidity levels, suggesting MWCNTs effectively impede $Sb_2Te_3$ oxidation, especially in humid conditions.

These results will not only enhance our comprehension of the impact of humidity on durability of thermoelectric substances but also play a vital role in the thermoelectric devices creation that operate efficiently in high-humidity environments. They will also help determine the optimal conditions for modifying materials to improve their resistance and durability in different climatic conditions.

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# Affinity Sensors Based on Conducting Polymers

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**Abstract ID #EN-1340**

Recently conducting polymer based structures are frequently used in the design of various sensors and biosensors. These conducting polymer based structures can be formed by electrochemical [1], chemical [2] and biochemical [3-5] methods. Electrochemical methods enables to modify electrodes by the conducting polymer layers which are suitable for enzymatic and affinity sensors [6,7]. The applicability of electrochemically generated polypyrrole in the design of electrochemical affinity sensors [1] will be discussed. Polypyrrole is well suitable for the immobilization of biomaterials, therefore, this conducting polymer is frequently applied in the design of affinity-sensors. Moreover, polypyrrole is suitable for the design of molecularly imprinted polymers, which can be used for the determination of different analytes including some biologically active molecules and biomarkers. Achievements of our research group in synthesis molecularly imprinted conducting polymers and application of these polymeric structures in the design of sensors for the determination of SARS-CoV-2 proteins will be addressed. The formation of conducting polymer based MIP layers by electrochemical methods will be presented [6]. Overoxidation of polypyrrole enables to improve the selectivity and sensitivity of MIPs. Advantages of molecularly imprinted conducting polymers in comparison to some other types of conducting polymers will be outlined [7]. Advantages and future trends in formation and application of conducting polymer based MIPs will be discussed.

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TRACK 4

# “MULTIFUNCTIONAL THIN FILMS & COATINGS”

# Analysis of the Surface Layer Stress and Strain State after Surface Plastic Deformation of Nanostructured Electro-Spark Coatings

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To increase the reliability and durability of machine parts, there exist many competing methods for improving the quality parameters of their surface layers. Among them [1, 2], a special place is occupied by the technologies using concentrated energy flows (CEF), owing to which there appear other surface layer structures being positively different from those created by traditional processing methods. Applying electrospark alloying (ESA) method with the use of special technological substance (STS), the compositions of which include nanoparticles of dosed amounts, there have been obtained the special coatings on Armco-iron, cast iron and alloyed steels, [3, 4]. There have been analyzed the mechanisms of nanostructure formation at the ESA method. There has been proposed a technology for combined surface treatment, which consists in the ESA method followed by surface plastic deformation (SPD) [5].

In this work, based on the results of the analysis of the stress and strain state of the ESA coatings, the equations for calculating the geometry and deformation parameters of the deformation zone are proposed taking into account the indicators of the coating obtained by the proposed technology. A general method for calculating the depth of the work-hardened layer and the strain intensity in the nanostructured ESA coatings with the uniformly distributed carbon nanotubes on the substrates made of Armco iron, cast iron, and alloyed steels has been developed, which allows controlling the quality of the surface layer of the essential parts within wide limits.

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# Low-Frequency Noises in MWCNT Films by Pulse Laser Deposition

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**Abstract ID #MTFC-0923**

The results of the study of excess noise in flat arrays of multi-walled carbon nanotube (MWCNT) are presented [1]. Thin films of nanocarbon were obtained by pulsed laser deposition (PLD). PLD is a process in which laser radiation is used to "punch" carbon materials from the surface layers of a target and deposit them on a substrate to form stoichiometric single and multilayer coatings with special properties [2]. A neodymium KGd(WO4)2 laser was used in the experiment.

Mechanical characteristics and physical impact are one of the methods of identifying a material, in particular its structure. The temperature dependence of the electrophysical parameters of the studied layers was also studied.

The excess noise was observed to be a superposition of the 1/f-like noise and the Lorentzian noise components of the recombination generation. The activation energies of the Lorentzian components and the distribution of the activation energies responsible for the 1/f noise were calculated from the measured temperature dependence of the noise power.

The calculated activation energies of noise components are in the range of energies of physical processes that are probably present in the studied carbon nanotubes. For example, fluctuations caused by carrier transitions between one-dimensional subbands will have an activation energy equal to the energy difference between the subbands [3]. It is possible that the noise originates from local defect centers because the semiconducting carbon nanotubes reduce the band gap. The Dutt–Horn model describes temperature-dependent low-frequency noise as thermally activated random fluctuations [4]. The saturation or even reduction of the noise at higher temperatures cannot be explained by this model. It was concluded that these processes are probably related to the sources of other low-frequency noise mechanisms.

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# Modeling of the Stress-Strain State in Multilayer Film Systems Depending on the Thermal Load

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**Abstract ID #MTFC-0933**

Applying nanocomposite nanostructured coatings to the surface of the contact zones of the metalworking tool, which are under the influence of significant thermal, physical-chemical and contact-force loads, increases their wear resistance, protects the tool from high temperatures and improves the corresponding tribological properties [1]. In our works the thermomechanical characteristics of TiAlN, TiCN/α-$Al_2O_3$ and TiAlN/α-$Al_2O_3$ film systems, three-layer TiC/$Al_2O_3$/TiN and TiN/$Al_2O_3$/TiC coatings were investigated. These coatings provide high heat resistance at high cutting speeds and sufficient wear resistance of the tool. The heat-shielding characteristics of these structures were studied [2, 3].

This work examines the effect of a nanoscale multilayer film system on the propagation of the thermal and strain-stress field in the cutting zone. Experiments were conducted that investigated the temperature field of a cutting tool plate made of 38XM (42$CrMo_4$) steel without a coating, with a single-layer coating of TiN, with a double-layer coating of TiN/α-$Al_2O_3$ under the influence of an external thermal load. Based on the obtained data, the temperature field inside the plate and its influence on the stress-strain states in it were analyzed, which in turn reduce the service life of the tool.

In the course of research, a significant positive effect of the use of coatings to increase the thermal stability of cutting tools was revealed. An uncoated surface indicates rapid heating and less thermal stability, which can lead to tool wear and reduced cutting quality. TiN coating and TiN/α-$Al_2O_3$ bilayer coating show improvements in these parameters, reducing temperature gradients and maintaining a more stable thermal field. It was established that the magnitude and law of temperature stress distribution, deformation processes in multicomponent systems are determined by the nature of the temperature field. Studies have shown that in the case of an uncoated thermal field, we see that the temperature gradients are high and the temperature levels are relatively higher near the heat source. This indicates rapid insert heating and potentially lower thermal stability, which can lead to tool wear and reduced cutting quality.

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# The Inhibitory Behavior of Eco-friendly Pigment Based on Montmorillonite Nanoreservoirs

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**Abstract ID #MTFC-0939**

The using of organic primer coatings is an effective anticorrosive method. They contain inorganic dispersed additives are known as pigments. Chromates are the most effective inhibitors for organic primer coatings. However, high toxicity and carcinogenesis limit their application [1]. An effective promising eco-friendly alternative is the using of pigments based on ion-exchange minerals, in particular, zeolites and montmorillonites, which are used as nanoreservoirs (containers) for loading of inhibitors in the anti-corrosion industry [2]. Montmorillonites are aggregates of lamellar platelets packed together due to the electrochemical forces. Each platelet consists of three sandwich-arranged layers: a central octahedral layer $Al_2O_3$ and two tetrahedral layers $SiO_2$. The aluminium cation often undergoes isomorphic substitution by lower valence metal, such as magnesium (Mg) and iron (Fe). This substitution leads to a negative charge imbalance, compensated by exchangeable cations, in particular $Na^+$, $K^+$, $Mg^{2+}$ and $Ca^{2+}$ as the most common ones [3]. Therefore, the aim of this study was to synthesize zinc loaded montmorillonite and evaluate the inhibitory effect of these nanoreservoirs on corrosion resistance of aluminium alloy.

Eco-friendly anticorrosive pigments based on zinc loaded montmorillonite for priming paint coatings were obtained by ion exchange method. Montmorillonite from bentonite clay was obtained by the coarse-dispersed phase sedimentation method. The surface morphology and chemical composition of initial and zinc loaded montmorillonites were determined by scanning electron microscopy and energy dispersion spectroscopy analyzes. It was established that a lamellar structure and the presence of $Na^+$ and $Ca^{2+}$ cations, with a predominant content of $Ca^{2+}$ cations of the initial montmorillonite. It was shown that the lamellar structure of the zinc loaded montmorillonite was preserved and the lamellae have had different shapes and sizes. According to potentiodynamic polarization results, it was established that the inhibitory efficiency of the Zn-montmorillonite extracts in an acid rain solution increases with an increasing concentration of the solution from which Zn-montmorillonite was obtained. The corrosion resistance of the aluminium alloy increases by 2-5 times compared to the uninhibited solution after 3 h immersion. The protective effect of the Zn loaded montmorillonite extracts is preserved during 168 h immersion. The degree of the inhibitory efficiency of aluminium alloy in an acid rain solution with synthesized Zn loaded montmorillonite extracts, after 168 h immersion, was more than 90%.

Consequently, modified zinc loaded montmorillonites are promising components for the production of the eco-friendly anticorrosive pigments for organic primer coatings.

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# Fabrication of SALDI-MS Chip with Au Nanoparticles/ZnO Nanorods for Sensitive Detection of Glutathione in Real Samples

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As an important bio-thiol molecule, glutathione (GSH) plays key roles in various cellular activities. However, it is still a challenge to analyze GSH in complex samples because of severe signal suppression from high abundance of interferent. The most efficient approach to tackle this problem is to enrich target analytes on-plate from the complex samples by selectively capturing and isolating [1].

Herein, the hierarchical substrates were synthesized for selective detection of GSH in real samples using surface-assisted laser desorption/ionization mass spectrometry (SALDI-MS) [2]. The structures are formed by homogeneously distributing Au nanoparticles (Au NPs) on ZnO nanorods (ZnO NRs). The Au NPs can selectively capture thiols through Au–S binding; ZnO NRs can not only efficiently absorb ultraviolet laser, but also isolate Au NPs–target compounds from complex samples as a carrier of Au NPs. Meanwhile, the Au–ZnO hybrid nanostructures can promote the hot electrons transfer at Au–ZnO interface and lead to higher desorption/ionization efficiency. The on-plate selective enrichment performance of the Au NPs/ZnO NRs as SALDI-MS substrates was demonstrated by successfully detecting GSH and L-Cysteine without interference peak in a mixed amino acids sample. The results in detecting GSH displayed high repeatability with relative standard deviation of 4.91 % for substrate-to-substrate, good linearity (R2 >0.99), and high sensitivity with the limit of detection of 150 amol. Furthermore, the Au NPs/ZnO NRs substrate is applicable for analyzing practical samples, such as GSH in medicine and fruits, which demonstrates its potential in practical applications.

## ACKNOWLEDGMENTS

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# Calorimetric Measurements of the Temperature of Metalic Targets During Magnetron Sputtering

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Direct measurements of the temperature of Cu, Ti, Cr targets (3 mm thick, Ø 55 mm) using thermocouples attached to the front (erosion zone) and back (cooling) sides of the targets during magnetron sputtering (DC MS) were carried. The variables: target mode (cooled or uncooled target); working gas (Ar, N2); discharge power per unit area. It was shown that the target temperature T(targ) reaches ~730 K on the front and ~530 K on the back sides of the cooled target, while for an uncooled target it is ~1050 K and 950 K, respectively (Cu target). For both modes and all targets, the T(targ) is slightly higher when sputtering in N2. The calculated target's surface temperature T(surf) doesn't depend on the target mode and target nature and substantially exceeds T(targ). e.g, the T(surf) ~1650 K, while the T(targ)~650 K (cooled Cu target). Based on temperature measurements on opposite sides of the Cu target, its dynamic thermal conductivity (thermal conductivity that exists during the target sputtering) is calculated. It turned out that it is ~100 times lower than the thermal conductivity of normal Cu. The above results are discussed using a physical model that assumes the appearance and existence during sputtering on the target surface of a layer whose properties are very different from those of ordinary metals.

## ACKNOWLEDGMENTS

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# Optical, Electrical and Gas Sensing Properties of the $MnCo_2O_4$ Thin Films

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**Abstract ID #MTFC-0990**

Transition metal oxides with a spinel structure attract attention in a wide field of research due to their unique magnetic, electrical, and optical properties. The sufficiently high electrical conductivity of $MnCo_2O_4$ promotes the use of the material for the creation of electronic devices [1]. In particular, $MnCo_2O_4$ thin films have been recognized as a suitable cathode material in hazardous gas sensors due to its high conductivity and tunable structural properties. Optical gas sensors for ethanol and acetone were created based on the optical properties of $MnCo_2O_4$ films [2].

Thin films of $MnCo_2O_4$ were produced by the spray pyrolysis method of a mixture of aqueous solutions of salts cobalt (II) chloride hexahydrate $CoCl_2 \cdot 6H_2O$ and manganese (II) chloride tetrahydrate $MnCl_2 \cdot 4H_2O$ with a concentration of 0.1 M at a ratio of components Co/Mn = 2. The pyrolysis temperature $T_S$ was 350 ºC. Compressed air was used as a carrier gas. Dielectric glass ceramics (1 cm × 2 cm) and transparent soda-lime glass (2 cm × 2 cm) were used as substrates. The $MnCo_2O_4$ films had a thickness of ~0.3 μm and had p-type conductivity. The contact pads on the films were created by depositing indium metal.

$MnCo_2O_4$ films have a transmission coefficient $T \approx 15 - 20$ % in the wavelength range $\lambda > 900$ nm. Analysis of the absorption spectra of the films indicates direct optical transitions. The optical band gap of the obtained $MnCo_2O_4$ films is $E_g = 1.3$ eV. As the temperature increases from 293 K to 383 K, the resistivity of $MnCo_2O_4$ films changes from $\rho \approx 533$ Ω·cm to $\rho \approx 20.4$ Ω·cm. The activation energy of the conductivity of the $MnCo_2O_4$ films $E_a = 0.31$ eV in the temperature range 293 K < T < 383 K indicates the ionization of acceptor levels in the band gap. The resistance of $MnCo_2O_4$ film samples, which were heated to temperatures of 323 K – 373 K, underwent changes in the environment of acetone or ethanol gases. The film resistance ($R_{gas} \approx 51$ MΩ) increased by an order of magnitude (at a film temperature of 323 K and at a volume concentration of 0.36 % acetone or ethanol) compared to the resistance under normal atmospheric conditions ($R_a \approx 6$ MΩ). The higher resistance of the films in the gaseous medium is preserved ($R_{gas} \approx 26$ MΩ and $R_a \approx 1.94$ MΩ) when the temperature of the films is increased to 373 K, with the same volume concentration of gases. The film resistance reacts to the presence of gas within about two seconds. The sensitivity of the electrical resistance of $MnCo_2O_4$ thin films produced by spray pyrolysis for gaseous media contributes to the prospect of their use as gas sensors. The value of specific electrical resistance of $MnCo_2O_4$ films is satisfactory for creating heterojunctions with other semiconductors.

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# Mechanisms of Formation and Modeling of the Structure of Films of Refractory Compounds

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**Abstract ID #MTFC-1005**

Transition metal films are widely used in the creation of micro- and nanoelectronics elements, as well as in manufacturing protective layers of various tools and parts. The analysis of previously conducted studies showed that, there are general patterns of their formation in the film state [1,2]. Films with a columnar structure have the best physical and mechanical characteristics [3]. To obtain films with specified properties, it is necessary to control magnetron sputtering parameters, for this, an understanding of the processes and mechanisms of film formation is required. Modern means of computer modeling provide significant support in understanding these processes [4].

In this work, the molecular dynamics method was used as it is more suitable for modeling the formation of critical nuclei at the initial stage. The 2NN MEAM multiatomic potential was used to calculate the interaction between atoms. The potential parameters for the Fe-Ti-N ternary system were proposed in [5], where their sufficient agreement with experiments was shown, in particular, the correspondence of the properties of the coherent interface between Fe and TiN.

Simulations of N and Ti atom deposition on an Fe(100) substrate were carried out using the MPI version of the open-source program LAMMPS (Molecular Dynamics Simulator). The substrate was modeled as a semi-infinite crystal with a frozen lower atomic layer, periodic boundary conditions at the lateral crystal sides, and a free deposition surface. The crystal size was 25 (length) × 25 (width) × 10 (depth) lattice constants, resulting in 18,900 Fe atoms in the substrate. N and Ti atoms were deposited one by one at random points on the central region of the (100) surface with a normal incidence angle. The size of this region was 7 × 7 lattice constants. The energies of the deposited atoms were randomly selected from 1 to 5 eV, and the atom type (N or Ti) was also chosen randomly. The time intervals between subsequent deposition events were either 10 or 5 ps in different simulations. Additionally, simulations were performed with either 200 or 500 deposited atoms. The substrate ambient temperatures were set to 500K or 1000K, maintained by the Berendsen thermostat.

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# Modification of gallium nitride defect structure by microwave radiation treatment for HEMTs, UV-LEDs and sensor applications

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**Abstract ID #MTFC-1013**

Gallium nitride is one of the best materials for high power electronics due to a wide band gap of 3.4 eV, a high breakdown field of 3.3 MV $cm^{-1}$, high electron mobility reaching up to 2000 $cm^2$ $V^{-1}$, a remarkable saturation velocity of 2.5 × $10^7$ cm $s^{-1}$, and high radiation tolerance. These properties are useful for high-power and high-frequency applications. In particular, for GaN-based high electron mobility transistors (HEMTs) with AlGaN/GaN epitaxial heterojunctions grown on different substrates, ultraviolet light-emitting diodes (UV-LEDs) [1] and high efficiency sensor systems [2]. The degradation mechanisms, including hot-electron induced degradation, charge-trapping, electrochemical oxidation and other are present at real exploitation of these structures. The presence of point and extended defects in the initial gallium nitride layer is always unwanted because all of them will increase of degradation risks [3]. That is why different approaches are used to decrease the levels of defects concentrations, including on post growth processes. In particular, microwave radiation processing [4] can be effective approach to modify initial impurity-defect composition of GaN before creation AlGaN/GaN epitaxial structure as well as $Ga_2O_3$/GaN heterostructure and improve initial structural perfection gallium nitride film.

Thermal annealing of point and extended defects in semiconductor material is well-known. But the heating of entire structure results in accompanied features related in the appearing of temperature gradient and enhancing diffusions impurities. Microwave radiation treatments is effective approach to modify defect subsystem of irradiated material. And neither temperature gradient no other unwanted processes not observed. The influence of microwave radiation treatment on defect concentration of promising GaN thin films which have incredible application in HEMT, UV-LEDs and sensor systems was investigated. Moreover, long-term features of defect subsystem evolution were established. Both spectral and structural methods were applied to obtain reliable results about defect concentration, in particular dislocations. To estimate evolution of defects level after microwave irradiation noted measurements were repeated during several days. Overall, the obtained results have the potential to advance our understanding of thin films defect engineering by microwave radiation treatment.

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# Light Metal-Containing Fillers for Polymer Composites

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**Abstract ID #MTFC-1014**

Many areas of science and technology require the use of materials that, along with certain specific properties, will also have low density and mass. At the same time, most of the fillers used to give polymer composites specific properties are usually characterized by high density, which affects the increase in the weight of the composite. In addition, their number must be significant to give the material the necessary properties, which also contributes to the increase in the density and mass of the resulting composite. Certain positive points can be achieved when using nano-sized fillers, which allow you to get the desired result with the introduction of a much smaller amount of filler. However, in the case of polymer composites, there are great difficulties with the process of introducing the nanofiller into the polymer matrix and its uniform distribution.

It is possible to propose another method of obtaining light polymer composites, which consists of using a relatively large amount of fine-dispersed micro-sized filler on the surface of which a thin coating is formed, which will provide the composite material with specific properties.

We have proposed the formation of a copper coating on polymer particles (polypropylene) by the method of chemical deposition. The technology involves the metallization of polymer particles in non-stabilized chemical reduction solutions of the following composition (mmol/l) $CuSO_4 \cdot 5H_2O$ - 60, EDTA-$Na_2$ ($C_{10}H_{14}N_2Na_2O_8 \cdot 2H_2O$) - 67, NaOH - 375, formalin - 365. Polymer loading density - 10 g/100 ml of solution. In order to obtain different copper contents on polymer particles, the method of repeated metallization was used. The already metallized polymer particles were placed in new portions of the chemical reduction solution. The resulting metallized polymer particles were used as filler in the preparation of epoxy composites.

The study of the density of the composites obtained shows that the filled composites are characterized by a lower density compared to the epoxy matrix. Even when using polymer particles with a copper content of 10% by weight, it was possible to obtain a composite material with a density close to that of cured epoxy resin. The production of epoxy composites characterized by low density and containing metal fillers in their structure is interesting from the point of view of the production of products with low mass. In addition, due to the presence of a metal filler, they will have a complex of interesting properties that can be used in a number of new industries and applications.

# Influence of Structure on the Properties of Coatings During Multi-chamber Detonation Spraying of $Al_2O_3$ Powder on Steel

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**Abstract ID #MTFC-1018**

Modern industry, including the energy, chemical, aircraft and space industries, uses products whose operational reliability depends on the characteristics of their surface layers. These parts and assemblies include the surfaces of combustion chambers, sealing connectors of prefabricated gas turbine housings, tension rollers for the paper industry, etc. To improve the performance and durability of products, various methods of surface treatment are used. The most promising is the application of functional coatings to their surfaces.

In the present work, we investigated coatings made of $Al_2O_3$ aluminum ceramics (AluminaTSP 99 Plus powder, fractions 5...30 μm), formed by the method of multi-chamber detonation spraying (MCDS). The multi-chamber design provides high velocities of detonation combustion products (1.8 km/s) and powder material movement (1.2-1.6 km/s). It has been established that a 300 μm thick coating with a porosity of 0.7...1.2% and a microhardness of 9660...11490 MPa is formed during the MCDS. Transmission electron microscopy studies have revealed features of the fine structure of the sputtered coating. A substructure with a size of 100...300 nm is formed in the coating material in the presence of nanoparticles with a size of 20...100 nm and a uniform distribution of dislocation density. The formation of the nanostructural state in the material of the obtained coatings is ensured by the technological parameters of the high-speed LBM process. This leads to a set of physical and mechanical characteristics of the surface layers of $Al_2O_3$ aluminum ceramics, namely, their strength and crack resistance.

# $AlNiCoFeCrTiB_X$ High-Entropy Coatings Prepared by Electron-Beam Cladding

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**Abstract ID #MTFC-1040**

Coating is considered one of the simplest and most widely used techniques for protection of the base metal. Some of the unique properties of high-entropy alloys (HEAs) for surface coating include high hardness and strength, excellent corrosion and oxidation resistance, remarkable wear resistance [1]. The coating of HEAs on metallic substrates can be achieved through different techniques including electron-beam cladding.

However, the strengths of simple-phased HEAs are usually limited. Among common strengthening mechanisms, second-phase strengthening is known to be the most effective [2]. Second phases can markedly enhance the mechanical properties of HEAs.

To improve the mechanical properties of the high-entropy coating on steel substrate boron element is added to form the boride phases as the strengthening phases. The $AlNiCoFeCrTiB_x$ (x = 0, 0.25, 0.5, and 1 mol) coatings were produced by electron-beam cladding and effect of boron element content on the microstructure and mechanical properties of $AlNiCoFeCrTiB_x$ coatings was investigated. When the content of the boron is x = 0 and x = 0.25, both coatings consist of two solid solutions with bcc1 and bcc2 structure and different lattice parameters. The addition of boron in amount of 0.5 and 1 mol promotes the in-situ formation of $TiB_2$ and $Cr_2B$ boride phases in bcc matrix solid solutions.

The Vickers hardness and yield strength of the $AlCoNiFeCrTiB_{0-1}$ coatings increase from 8,8 to 14 GPa and from 2440 to 4040 MPa, respectively, and the strengthening effect reflects a significant positive effect of boron. The coatings strength characteristics enhancement can be attributed to the effect of solid solution strengthening and to the precipitated strengthening of boride phases in the coating structure.

Thus, this result opens broad prospects for the further production of high-entropy coatings and alloys with significantly improved characteristics by boron dopant.

This study represents first step to develop the electron-beam coatings of given composition for various purposes and characteristics by changing the boron content. In addition, it is advisable to further investigate the effect of changing the elemental composition of a high-entropy coatings/alloys and a variety of traditional and new methods of obtaining.

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# Effect of the Surface Nanocrystallization on the Gas Nitriding of Two-Phase Titanium Alloy

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**Abstract ID #MTFC-1041**

Due to their excellent mechanical and anti-corrosion properties, the aircraft industry widely uses high-strength two-phase titanium alloy (Ti–5Al–5Mo–5V–Cr–Fe, so-called VT22). However, this titanium alloy has low wear resistance, which limits its use in tribo-pair without additional surface treatment and, therefore, determines the need to develop effective surface engineering methods [1, 2]. For these reasons, gas nitriding is a promising, technologically simple, and economically efficient surface engineering method for wear resistance enhancement of titanium alloy. Generally, the treatment temperature for conventional gas nitriding of titanium alloy is near 950°C, with a processing time of several tens of hours. This results in high-energy consumption and significant adverse effects on mechanical and fatigue properties due to the growing grains of titanium alloy's matrix microstructure. Therefore, the issue of intensification of nitriding of titanium alloy becomes especially relevant [2-4].

Our study shows the intensification of gas nitriding by pre-surface nanocrystallization titanium alloy. Diamond ball burnishing was used for surface nanocrystallization. By carrying out pre-surface nanocrystallization, it is possible to activate nitride formation on the surface of the titanium alloy, which leads to the texturing of the nitride layer from the nitride of lower valence Ti2N into mononitride TiN. The intensification of nitriding is evidenced by an increase in surface microhardness (50%) and a thickening of the hardened layer (30%) compared to conventional gas nitriding under similar time-temperature parameters but without pre-burnishing. This intensification can be attributed to high-density dislocations and grain boundaries introduced by pre-nanocrystallization, which served as efficient channels for nitrogen diffusion.

In summary, we can conclude that pre-nanocrystallization intensifies the gas nitriding of the titanium alloy, makes it possible to reduce the time-temperature parameters of treatment, and forms new surface layers with higher functional characteristics.

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# Sensors Based on Hybrid Materials for Environmental, Industrial and Biomedical Applications

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**Abstract ID #MTFC-1082**

Technological advancements are in high demand in both the industry and healthcare sectors. To effectively adapt technologies to specific needs, understanding processes and receiving accurate feedback is crucial. Developing different sensors, such as metal oxide semiconductor structures, can cater to economic and technical demands. These sensors can be adjusted through various methods and processes, including doping with metals or coating with polymers, resulting in hybrid structures that enhance sensor characteristics.

For instance, a recent study [1] presented a 15 nm thin film of TiO2 coated with PV4D4 polymer, which showed good selectivity towards 2-propanol at different temperatures, with the highest response value of about 220% at 400 ºC. 2-propanol has a potential link to lung cancer, which is the subject of ongoing research [2], making more room for new methods to detect it in its early stages. For the same reason, another TiO2 sample coated with a PTFE polymer was studied, which also showed a new approach in detecting 2-propanol [3] at 350 ºC operating temperature with a response value of 45%.

Similarly, hybrid material-based sensors have the potential to be developed as "two-in-one" sensors, as in another study [4], where a TiO2 sensing nanostructure pre-annealed at 610 ºC and coated with PV4D4 showed an about 50% response at 100 ppm ammonia at room temperature and high selectivity at relatively higher operating temperatures for hydrogen, with a 100% response value at 300 ºC. This study promotes a new direction in the development of dual-use sensors, as ammonia detectors could be used in the diagnosis of kidney failure and the same sensing structure could be used for food spoilage by detecting both ammonia and hydrogen.

Another field of application for hybrid sensors would be the early detection of hydrogen gases in Lithium-Ion Batteries (LIBs) or of the gases that are produced as a result of the reactions of the electrolytes in them. These require strict monitoring and at the right time disconnecting the batteries from the system to reduce the effect of thermal runaway. Thus, sensor heterostructures based on CuO/Cu2O/ZnO:Fe coated with PV3D3 polymer, selective to H2 gas with a high response of about 200% and excellent stability at relative humidity (RH) were obtained [5].

All these experimental results enables updated possibilities in application fields like medical diagnosis, bio-sensors, industrial and the development of non-invasive technology and environmental safety.

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# Encapsulation Layer Stalilized 2D $WTe_2$ Materials

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2D Transition-metal dichalcogenide (TMDC) monolayers have been extensively studied over the past decade and are well known for covering a wide range of properties from insulators and semiconductors, therefore they are promising for a rich variety of applications in electronics as transistors, in optics as emitters, detectors[1], and many more. Recent findings of exotic topological insulator properties in one of the TMDC materials - tungsten ditelluride have further broaden application range in spintronics, memory devices, and exotic applications relying on properties of topological surface and edge states. $WTe_2$ also exhibit an extremely large magnetoresistance and its monolayers can be turned superconducting[2]. Majority of future applications rely on stable charge transport characteristics, however, 2D $WTe_2$ is particularly prone for adsorption of oxygen and water, which interacting chemically, result in rapid surface oxidation[3].

Here we study innovative polymer protecting layers that effectively isolate 2D $WTe_2$ monolayers from ambient environment components such as oxygen and water, therefore considerably slowing down its degradation. We found that perhydropolysilazane (PHPS) shows excellent barrier properties against water vapor and oxygen, and it has low electrical conductivity, therefore making it suitable candidate for different applications in field of 2D TMDC electronics. A method for applying PHPS coatings was developed and the optimal parameters for the curing of PHPS coatings were determined. Coated 2D $WTe_2$ structures were studied using Raman and FTIR spectroscopy methods, as well as carrying out charge carrier transport measurements at low temperatures. Our results show that inorganic polysilazane can be used to coat $WTe_2$ structures efficiently and protect them from the destructive effects of the external environment.

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# Multilayer Interference Mirrors with Nanoscale Metal Layers

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**Abstract ID #MTFC-1093**

Interference coatings have found wide application in optical instrumentation, including laser technology. In particular, high-power technological CO2 lasers use cavity mirrors with interference coatings, which make it possible to achieve a reflectivity very close to 1 at a certain wavelength. Typically, multilayer coatings of alternating transparent dielectric layers with the most different refractive index (dielectric mirror) are used for this purpose. Such an interference (dichroic) mirror reflects one and transmits another part of the spectrum of incident radiation due to the phenomenon of multipath interference in thin dielectric films. The exact values of the layer thickness determine the position of the maximum of the transmission curve, while the width of the filter's passband and the degree of suppression of the unnecessary part of the spectrum depend on the number of layers.

The fabrication of interference mirrors is quite complex because it requires at least two sources to deposit different materials. At the same time, it is possible to create dichroic mirrors with alternating layers of a transparent dielectric (¼ wavelength thick) and transparent metal (several nanometers thick). If reactive sputtering is chosen as a production technology, then only one target may be used for the deposition of both types of layers.

In this research, interference mirrors based on "tantalum oxide/tantalum" multilayer structures were experimentally produced and studied. Ta2O5 films are hard and have high chemical stability. The films are transparent in the visible and near UV and IR regions. High-quality transparent Ta2O5 films were synthesized by reactive magnetron sputtering of a metal tantalum target with additional activation of the reactive gas using a dedicated inductively coupled plasma source. The alternation of metal and dielectric layers was ensured by opening/closing the oxygen flow using a mass-flow controller guided by a precision timer. All samples contained 20 layers (10 layers of Ta and 10 layers of Ta2O5) with constant thickness. The metal and dielectric layer thickness varied sample-to-sample to change the shape of the reflectance spectrum, which was measured using a spectrophotometer in the wavelength range 200-1000 nm.

It was shown in the experiments that by changing the thickness of the dielectric layers, it is possible to shift the passband and stopband within the entire optical spectrum, and changing the thickness of the metal layers allows you to adjust the width and depth of the passband. Based on the results of the research, it can be concluded that tantalum-based interference coatings can be used for practical applications as optical and decorative coatings due to their durability, weather resistance, and low absorption in the operating wavelength range.

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# Annealing Effect on Structural and Mechanical Properties of Atomic Layer Deposited $Cr_2O_3$ Films Doped with Ti and Al

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**Abstract ID #MTFC-1109**

One of the important trends in the development of novel electronic devices is related to the application of oxide thin films. Among them, chromium oxide ($Cr_2O_3$) due to its chemical stability, mechanical strength, and optical characteristics has attracted marked interest in recent years. Previous research has indicated that doping chromium oxide with appropriate elements allows tailoring the electrical, mechanical, optical, and oxygen diffusion-barrier properties [1,2]. The effect of annealing treatment on structural, mechanical, and optical characteristics has been often the focus of the research [3].

In the current study, we investigate the microstructure, density, thickness, and surface roughness in a variation of annealing temperature up to 900 °C of undoped $Cr_2O_3$ films and those doped with aluminum (Al) and titanium (Ti) deposited by ALD on Si (100) substrates. In-situ high temperature X-ray diffraction and nanoindentation measurement were used for structural characterization and mechanical properties of the films, respectively. The increase in the hardness of the $Cr_2O_3$ films from 14 GPa to 15.2 and 17.5 GPa was observed when doping with Ti and Al, respectively. Changes in microstructure and crystallinity were observed starting from 500 °C for undoped $Cr_2O_3$ film, however, no remarkable changes were observed in phase composition and densities of the doped films with Ti/(Ti+Cr) = 0.26 and Al/(Al+Cr) = 0.29 when annealing up to 900 °C. The formation of an intermediate layer between the substrate and the film with a thickness of ~11 nm was observed for $Cr_2O_3$ film at 900 °C, however, a similar situation was not observed for the doped films which can be explained by the suppression of oxygen diffusion in the doped films. Our results demonstrate the significant impact of doping of atomic layer deposited ultra-thin $Cr_2O_3$ films (thickness $\leqslant$ 50 nm) on increasing hardness and thermal stability, but also inhibiting oxygen diffusion all of which are important features for various applications in industry such as protective coatings at high temperatures.

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# Increasing the Productivity of Electron Beam Evaporation of Ag and Cu Antimicrobial Nanocoatings on Mg-Based Alloy Implants

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**Abstract ID #MTFC-1127**

One of the urgent tasks of today is the development of new types of implants for osteosynthesis, and a promising material for this application is magnesium alloys, which have high biological compatibility, mechanical properties close to the properties of bones, as well as the ability to biodegrade over time, which eliminates the need for repeated surgery to remove the implant [1-2]. We developed an experimental alloy of the Mg-Ga-Zn-Ca system, which showed improved physical and mechanical properties and an acceptable corrosion rate for this application. At the same time, it is important for any implant to prevent the introduction of bacteria and viruses during the operation, which significantly worsens the pace of medical treatment and can lead to serious complications. Thanks to the size effect, nanoparticles have unique properties that allow them to be used as components of modern materials for biomedicine. Research is being conducted in the areas of diagnostic, therapeutic and prophylactic use of Au, TiO, Ag, Cu, Zn, Si, CeO, Pt nanoparticles [3-4].

The analysis of approaches to the synthesis of Ag, Cu nanoparticles showed the advantages of the synthesis of nanoparticles by methods of physical deposition in a vacuum over methods of chemical and hybrid synthesis [5]. We have developed a scheme with a new variant of the evaporator with the ability to form an intense vapor flow of the material being evaporated (Ag, Cu) in a selected direction, which allows to reduce the consumption of material by 6-10 times compared to the traditional "crucible" scheme of evaporation. The optimal technological modes of deposition from the evaporator to achieve homogeneity of the directional steam flow were determined. The dependence between the temperature of the target, the efficiency of the evaporation scheme and the distance of the evaporator from the target was determined experimentally.

It was established that an evaporator with a "vertical" orientation of the steam pipe, in comparison with an "angled" one, provides a higher efficiency and has a higher homogeneity of the distribution of the steam flow on the surface of the target, which gives a higher value of the reproducibility of the process of synthesis of nanoparticles. It was determined that when applying this technological scheme, for the evaporation of silver and copper with subsequent deposition and formation of a uniform layer of antimicrobial nanocoating on the surface of the developed magnesium alloy, it is possible to ensure a high efficiency of up to 20% at the following optimal parameters: distance to the substrate 80 mm, current strength 0,03 A, evaporation rate 5 mg/min.

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# Structural and Optical Properties of Composite and Multilayered Si-doped $HfO_2$ films

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**Abstract ID #MTFC-1138**

"High-k" hafnia and its silicates are considered mainly as promising candidates to replace $SiO_2$ in microelectronic devices due to minimal tunnelling current, a good thermal and chemical stability, as well as good interfacial quality with Si channel. Different research groups reported on a crucial role of the fabrication approach on the structural properties of $HfO_2$ films that are known to be crystallized at 300-350 °C. Except this drawback, $HfO_2$ shows higher refractive index than $SiO_2$ that is attractive for its optical applications, for instance, for waveguides. Thus, the stabilization of amorphous structure of $HfO_2$ films at higher temperatures is challenging.

Among different fabrication approaches, the most promising is the film deposition under non-equilibrium conditions and radio-frequency magnetron sputtering becomes the most attractive technique. Earlier we reported on the improved stability of ultrathin $HfO_2$ films doped with 3 at.% of Si. In this work, the effect of Si content in wide range (up to 20 at.%) on the structural and optical properties of thick films is considered. The deposition was performed on Cz-Si and fused $SiO_2$ substrates in argon and argon-hydrogen atmosphere by sputtering of composite Si-$HfO_2$ target. To effect of RF power density, substrate temperature and argon-hydrogen partial pressure on optical properties and morphology of the films was investigated by means of photoluminescence, ellipsometry, FTIR spectroscopy, TEM and Scanning Auger microscopy methods.

It was found that the increase of Si content up to 20 at % increases the refractive index of silicate films up to 2.42 (taken at 632 nm) against 1.98-2.00 obtained for pure $HfO_2$. Besides, the films with the thickness from 200 up to 700 nm demonstrate amorphous structure and homogeneous chemical composition not only in as-deposited state, but also after annealing at 400-900 °C in nitrogen atmosphere. This is an evidence of the thermal structural stability of such films that make them attractive for optical applications. An annealing at 1000-1100 °C favors the phase separation and the formation of $SiO_2$ and $HfO_2$ phases. The crystalline structure of the latter was found to be monoclinic one for [Si]<6 at.% and tetragonal one for higher Si content. This phenomenon was assumed to be caused by the presence of some residual Si atoms in $HfO_2$ phase.

The fabrication of the films with high RF power and in argon-hydrogen plasma permits to achieve high Si content. Taking into account this phenomenon, the alternative sputtering of the target in pure argon plasma or in mixed argon-hydrogen plasma was performed and multilayered structure of the films was achieved. This was evidenced by TEM and Scanning Auger Microscopy methods. The effect of thermal treatment on the phase separation in such multilayered films will be discussed in details to show the possibility to obtain specific red emission due to Si clusters formation that can offer also their photonic application.

# UV irradiation Impact on Structuring of Films Modified with Epoxy Resin

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**Abstract ID #MTFC-1150**

The structuring of protective coatings under the ultraviolet (UV) influence has the great importance due to the use of oligomeric and oligomer-monomer systems allowing to form high-quality films practically without the volatile components release in a quit short time. Epoxy resins- based films under UV irradiation are able form chemical-, moisture- and atmospheric-resistant coatings of high dielectric properties.

The formation of spatially cross-linked structures based on epoxy resin occurs in the presence of a photoinitiator. The role of last one is to provide with the possibility of both radical and cationic polymerization proceeding in the system. This enables a single three-dimensional mesh structure formation that has sufficient operational characteristics of films based on epoxy resin.

Research were conducted concerning the possibility of forming of polymer films based on epoxy-oligoester compositions under the UV radiation impact. The possibility of UV irradiation using for the formation of insoluble films based on epoxy-oligoester compositions in a relatively short time (no more than 10 min) has been showed; the obtained products regarding the number of spatially cross-linked structures, practically do not differ from the products obtained by the structuring method at the room temperature, followed by prolonged heating.

Studies have demonstrated that compositions containing the ED-20P peroxide resin, as well as in its absence are able to form polymer products with a spatially cross-linked structure under UV radiation in a relatively short time. In the case of mixtures containing peroxide resin the gel fraction content reaches 95% for 10 minutes.

Peroxide resin significantly affects the formation of three-dimensional structures. To study the influence of UV rays on the formation of three-dimensional structures the studies in which UV rays were cut off applying the silicate glass were conducted. This slowed down the process. The three-dimensional structure products formation in the absence of irradiation is being observed only after 8 minutes. However, the gel fraction content makes 40% in the case of cut-off and 82% in the case of radiation effect on the film.

Thus, the conducted studies showed the possibility of applying UV irradiation for insoluble films based on epoxy-oligoester compositions formation. This method allows in a relatively short time to obtain compositions that, in terms of the number of spatially cross-linked structures, practically do not differ from those obtained by the method of structuring at the room temperature with further prolonged heating.

# Nanostructured Thin Films with Nanocolumns and Nanoparticles: Sputtering-Based Manufacturing and Recent Applications

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**Abstract ID #MTFC-1156**

In this talk, it will be shown that nanostructured films with nanocolumns and nanoparticles can be fabricated using methods based on magnetron sputtering, which is of particular interest from an industrial perspective. Several applications of these films will also be presented.

In the first part of the talk, physical methods in ultra-high vacuum based on magnetron sputtering, used to prepare nanocolumns and nanoparticles, will be briefly explained: nanocolumns are fabricated using the glancing angle deposition (GLAD) technique [1], while nanoparticles are produced using a multiple ion cluster source (MICS) [2]. Both GLAD and MICS techniques will be discussed in terms of control over chemical composition, shape, and dimensions of the fabricated nanostructures. It will be argued that these are environmentally friendly techniques since they are carried out at room temperature with moderate energy consumption, do not involve chemicals (i.e., no recycling issues), and allow for the production of nanostructured surfaces of considerable size (several square centimeters in the lab) with high purity, making them quite appealing for industrial applications (scaling-up is feasible).

In the second part of the talk, several applications of these nanostructured films will be presented, both with homogeneous films (for example, for effective chemical detection using enhanced surface spectroscopies [3] and as magnetic surfaces [4]) and with heterogeneous films that combine nanocolumns and nanoparticles, highlighting the benefits of that combination. In particular, it will be shown that heterogeneous films can be used as surfaces with photo-induced self-cleaning activity [5], and as dual-scale roughness structures for wettability control (preliminary results of ongoing experiments).

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# Developing High Y Content TiAlYN Coatings: Structure and Adaptive Tribological Behavior

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Dry high-speed machining has become increasingly important in recent years due to its potential to reduce production costs and environmental hazards. Coatings used in dry cutting applications need to have excellent resistance to oxidation. The properties of TiAlN-based coatings can be improved by adding alloys such as Y, Cr, Zr, V, Si, B, and Hf. The addition of yttrium to TiAlN-based coating plays a significant role in enhancing mechanical properties and oxidation resistance. This happens because yttrium is segregated during film growth, leading to grain refinement and the formation of a protective film due to its strong affinity for oxygen. The addition of yttrium also boosts the coating's hardness and mechanical properties, although it reduces compressive stress [1]. Despite exposure to high temperatures, the TiAlYN coating maintains its hardness, demonstrating increased resistance to wear and corrosion [2]. While much valuable data has been reported on the deposition of TiAlYN coatings, the impact of a high Y-content on their structural nuances and tribological behavior is still relatively unclear. Conducting research in this area could pave the way for the creation of more efficient Y-containing coatings that can be utilized in high-performance industrial applications.

Here, we report on the high Y content TiAlYN coatings deposited by the cathodic arc evaporation method from sintered cathodes with two chemical compositions (Ti45Al51Y2 and 4Ti45Al51Y4) in an N2 gas atmosphere. The addition of Y (2-4 at.%) does not alter the phase structure of the TIAlN coating, which is a mixture of fcc-TiN (JCPDS No. 00-038-1420) and fcc-AlN (JCPDS No. 00-025-1495). The preferred orientation is strong in {200}. The atoms of Y dissolve into the AlTiN, forming a solid solution instead of segregating as a second YN phase. The dissolution of Y into the Al-Ti-N lattice increases the lattice parameters of the TiAlYN coating because Y has a larger atomic radius than Ti and Al. However, after Y addition a broadening of the characteristic peaks of the solid solution TiAlYN can be observed, which can be attributed to the grain refinement. The higher Y content in TiAlYN coating exhibits significantly improved wear resistance compared to the Y-free and 2at.%Y-containing coating. The improved tribological parameter is attributed to the dense and refined grain microstructure and the retardation of the cation caused by the addition of Y. Consequently, the wear resistance of the coating is improved, owing to grain refinement and densification. In experimental wear tests, the addition of Yttrium promoted the formation of Y2O3 and Al2O3 films and improved the interface bonding between the oxide layer TiAlYN coatings..

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# Effect of Heat Treatment Over the Mechanical and Tribological Properties of the Cr/DLC Coating

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**Abstract ID #MTFC-1166**

Diamond-Like Carbon (DLC) coatings possess both sp3-and sp2-bonded carbon which make it to have excellent mechanical, tribological, electrical, and optical properties. DLC films can be amorphous, hard and strong based on the composition and synthesis process. However, high residual stress within the film leads to poor adhesion to the substrate materials and it restricts its potential applications in many areas. Some common methods to reduce the residual stress is to increase the deposition temperature, post-synthesis annealing and vacuum furnace heat treatment method. In the present study, Cr/DLC bilayer thin films were synthesized using a DC magnetron sputtering system over Silicon (100) substrates. Prior to the synthesis the mechanical properties of the deposited film were characterized by nanoindentation test. From the nanoindentation, the hardness (H) and Young's modulus (E) of the coating were calculated. Stoney's equation was used to find the residual stress of the developed coating. A vacuum furnace was used for the heat treatment of the Cr/DLC coating at different temperatures ranging from 180 ºC to 300 ºC. After the heat treatment, the coating was again characterized by nanoindentation to find out the mechanical properties like H and E. Stoney's equation was again used to find the residual stress of the heat-treated Cr/DLC coating. The results showed that the residual stress of the coatings was significantly decreased with the increase of the heat treatment temperature up to 270 ºC. However, the residual stress of the coating heat treated at 300 ºC was slightly decreased compared to the decrease of the H and E of the coatings.

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# Structure and Hardness of Detonation Coating Based on Fe-$Tib_2$-$Crb_2$ after Pulse-Plasma Treatment

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**Abstract ID #MTFC-1169**

This paper presents the results of a study of the effect of pulsed plasma treatment on the properties of Fe-$TiB_2$-$CrB_2$ eutectic alloy coating, such as phase composition and hardness, roughness. This coating was deposited using a multi-chamber detonation machine followed by modification by pulsed plasma treatment. Mechanical tests revealed that the hardness of the coating increases after pulse plasma treatment. According to X-ray diffraction analysis, the increase in hardness is attributed to phase transformations in the surface layer, including the formation of oxide phases and an increase in the number of carbide phases.

## ACKNOWLEDGMENTS

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# The Effect of Lanthanum and Yttrium Doping on Photocatalytic Properties of ZnO Ffilms

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**Abstract ID #MTFC-1170**

The doping of ZnO using rare earth elements (REE) is promising approach for improving its photocatalytic efficiency. REE incorporated into ZnO films changes its electronic band structure and as a result, modify its optical properties and enhanced photocatalytic effect. But, the most of papers is related to the synthesis of ZnO nanoparticles. The photocatalyst in the form of thin films has the advantage that it can be easily separated after the photocatalytic reaction, which eliminates the problem of ZnO release into the environment [1, 2].

Undoped and La(Y)-doped ZnO films were grown by radio frequency magnetron sputtering on silicon substrates using the universal vacuum unit UVN-70 in an Ar atmosphere at a power of 200 W. The oxide powders were mixed with the ratios of ZnO/La2O3(Y2O3) = 5 and 10 % wt. Substrate temperature was established at 350 °C. Sputtering time was 30 min.

The photocatalytic activities of the samples were evaluated by photocatalytic degradation of Methyl Orange (MO) under Hg lamp irradiation. Undoped and La(Y)-doped ZnO films, immersed in MO solution, were exposed under irradiation for 60, 120, and 180 min, respectively.

The reaction rate constants (k) were calculated from the slopes of the plots ln(C0/C) versus the time of irradiation (t) for each sample. It can be found that the reaction rate has improved after doping ZnO by La3+ and Y3+ ions compared with undoped ZnO films. For undoped ZnO films, the value (k) consists of 0.916 min-1. For La-doped ZnO films (5 and 10 % wt.) the calculated values of the degradation rate constant (k) are 1.99 and 1.40 min-1, respectively. For Y-doped ZnO films (5 and 10 % wt.) the values (k) are 1.52 and 1.47 min-1, respectively.

The degradation efficiency (DE) of REE-doped ZnO films was improved compared to undoped ZnO films (30 %). The La-doped ZnO (5 % wt.) demonstrated the higher photodegradation efficiency (51 %) than samples with 10 % wt. (39 %) after 360 min exposure to irradiation. The DE of ZnO with 5 % wt. Y3+ is slightly higher (42 %) than for samples with 10 % wt. (40 %) dopant concentration. Therefore, La- and Y-doped ZnO films exhibited higher photocatalytic activity than undoped ZnO films. The increasing of La2O3(Y2O3) impurity up to 10 % wt. leads to reducing the photocatalytic efficiency of ZnO films compared to 5 % wt. doped. The reducing in photocatalytic activity with a further increase of ZnO doping up to 10%wt., can be related with the formation of a larger number of chemical bonds in the crystal structure, that negatively influences on efficiently separation of the photoinduced electron-hole pairs. It can be concluded that the optimal dopant concentration of lanthanum and yttrium is about 5 %wt.

Presented results indicate that La(Y)-doped ZnO thin films are promising photocatalytic materials for the practical use in the photodestruction of organic dyes.

## ACKNOWLEDGMENTS

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# Thickness Induced (Micro/Nano) Structuring of a-C Thin Films Deposited by Radio-Frequency Sputtering

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**Abstract ID #MTFC-1173**

Amorphous carbon (a-C), fascinating group IV element, have stimulated great interest from both scientific and industrial perspectives owing to its tunable optical band gap and potential applications in micro- to nano- electronic devices. In this work, a-C films have been deposited over Si(100) substrate by RF sputtering technique of varying thickness. Thereafter, these films have been ex-situ annealed at a temperature of 500°C for one hour in argon atmosphere. The effect of film thickness and ex-situ annealing on the microstructure and optical energy gap of carbon films has been studied systematically. The optical energy gap follows increasing trend with increase in film thickness and annealing. Differences in the microstructure of the amorphous carbon (a–C) films in terms of sp3 and sp2 content has been used to explain the tuning of optical characteristics of these sputtered films.

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# Formulation of 2K Epoxy Adhesives with Addition of Electrochemically Exfoliated Graphite for Joining Magnesium Fire Protection Boards

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One of the most frequently used methods of polymer modification is the use of carbon nanomaterials as additives. An example of one of the interesting directions of development is the formulation of adhesives using nanocarbons [1,2]. 2K epoxy resin-based adhesives for joining magnesium fire protection boards used to protect reinforced concrete structures were designed. The composition of such adhesives, apart from almost 50 wt% of inorganic fillers, included 0.5, 1, or 1.5 wt% of electrochemically exfoliated graphite (EEG) synthesized from polycrystalline graphite in a process including oxidation, anion intercalation, and anodic exfoliation. The developed adhesive compositions were characterized using selected methods of thermal analysis, such as differential scanning calorimetry, thermogravimetry, and cone calorimetry. The change in the value of the water contact angle (CA), surface free energy (SFE), and the color of the cross-linked adhesives (CIELab) were also assessed. It was observed that even the addition of 1.5 wt% of EEG does not lead to a noticeable change in the analyzed properties of adhesive compositions. All tested variants were characterized by similar thermal stability. 5% weight loss occurred at 270-277ºC for the reference sample and with 1.5 wt% EEG, respectively, and the glass transition temperature was approximately 130ºC for all compositions. Interestingly, it was reported that the presence of EEG results in an increase in heat release rate. CA of 73-77º and SFE of approximately 44 mN/m were recorded. The color of the adhesives changed from L* = 68.07, a* = 0.43, b* = 6.50 to L* = 30.86, a* = 0.02, b* = -0.30, which gives a color change of ΔE = 37.83. Therefore, future laboratory research will be based on increasing the EEG content in adhesive compositions up to 2.5, 5, and 10 wt% and the repetition of carried tests with the extension with strength tests.

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# Searching for the Dependence Between the Type of Pigments and the Selected Properties of Coatings During Aging Tests

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**Abstract ID #MTFC-1184**

The primary function of protective coatings for steel constructions is twofold: to offer long-lasting defense against corrosion and to preserve their decorative qualities over extended periods of use. Obtaining these goals is possible by appropriate selection of topcoat materials, i.e. those that ensure the durability of key functional properties during exploitation. Although there are several technical requirements and standards for assessing colour stability for powder coatings, e.g. Qualicoat, Qualisteel, AAMA, and GSB [1], in the case of liquid products there are no such documents with guidelines. The main goal of the project is to investigate the impact of cyclic changes in temperature, humidity, and UV radiation intensity on the properties of topcoats. And based on the results obtained, find out whether it is possible to indicate a scheme of conduct including the selection and methods of modifying paint components to extend their life. Polyurethane paints pigmented in various shades of yellow, red, and blue, using both micro and nanometric pigments, were tested. Via Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), goniometer, glossmeter, and colorimeter, the following were assessed: stability of colour, gloss, water contact angle, and surface energy of coatings during exposure to xenon and UV lamps and after tests in climatic chambers. It has been shown that exposure to UV radiation has the greatest impact on the change in the above properties, including maintaining the decorativeness of topcoats. Subjecting coatings to changes in humidity and temperature showed less impact. Thanks to FTIR analysis, it was possible to track the progress of the degradation process of the polymer binder used [2], which was reflected by a change in the morphology of the coatings imaged using SEM. Completing all the tests planned to be performed will enable the preparation of a rich file dealing with the interdependence of the tested binder-pigment systems and the durability of coatings in changing climatic conditions imitating the operational environment. Such a description will be of great value, especially from a practical point of view.

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# Investigation of the Effect of the Chemical Composition of Thin Nanostructured Films of Ni-Cu Alloys on the Structure, Electrical and Magnetic Properties

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**Abstract ID #MTFC-1195**

The article presents the results of a study of the effect of the chemical composition of thin nanostructured films of Ni-Cu alloys on their crystalline structure, electrical and magnetic properties.

Thin films of Ni-Cu alloys were obtained by simultaneous evaporation of pure metals in vacuum from two independent sources at a residual atmospheric pressure of $10^{-5}$ Pa. The purity of the evaporated metals was no less than 99.98%. The condensation rate was 0.5-1.5 nm/s. The thickness of the films was measured using a computerized microinterferometer MII-4. The thickness measurement error was 5-10% for thicknesses of 50-200 nm and 10-15% for thicknesses d < 50 nm. To determine the concentration of components, the calculation method and the method of X-ray microanalysis (scanning electron microscope REM-103-01 and spectrometer with energy dispersion of EDS) were used. A comparison of the results shows that in the region of film alloy thicknesses d < 100 nm, the discrepancy between the calculated and measured concentration values is about 10%. For sample thicknesses d > 100 nm, the discrepancy decreases to 1-3%. Film alloys of all studied thicknesses and concentrations have an fcc lattice with a parameter that depends on the concentration of the components and varies from a = 0.352 nm to a = 0.362 nm. The obtained dependence of the fcc lattice parameter of alloy films on the concentration of components is generally consistent with Vegard's rule. Concentration effects in the electrical conductivity and TCR of film alloys have been established. As for massive alloys, the concentration dependence of resistivity is observed to pass through a maximum (for TCR – through a minimum), although both of them are shifted by 10 at.% towards a decrease in copper concentration. The magnetoresistance of samples with different concentrations of components was studied. It was found that for all samples with a copper content of more than 35 at.%, even at a temperature T = 150 K, the effect of magnetoresistance was practically not observed. This indicates the absence of a domain structure in them.

# Resistive Sensitivity of Nanocrystalline Copper Oxide Films to Ammonia Vapors

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**Abstract ID #MTFC-1200**

Detection of volatile organic substances (VOC) is an important task of modern technologies. It is necessary to improve life safety, control the operation of technological processes and prevent man-made disasters. An important element in solving this applied problem is the development of new thin-film devices that combine compactness and low cost. Also, the problem of VOC detection is the need to heat the sensor, which is particularly dangerous in many production facilities. Nanocrystalline composite films can help in solving this problem. Such structures, due to their internal and external boundaries, can provide sensing mechanisms not available to the bulk state. In this regard, this work is devoted to studying the effect of ammonia vapor on the resistivity of CuO/$Cu_2O$ nanocomposite films and developing a prototype ammonia sensor that can operate at room temperature.

Samples for the study were preparation as follows. First, copper films of 50 or 100 nm thickness were deposited by thermal vacuum evaporation. Two series of samples of each thickness were prepared. Samples of one series were deposited on substrates at room temperature. Samples of the second series were deposited on substrates at 250°C. After deposition, they were incubated for about one hour. After that, the films were annealed in air for 20 minutes, due to which their oxidation took place.

Using optical transmission and reflection data, it is shown that the films obtained in this way are composite and consist of two phases CuO and $Cu_2O$. According to elemental analysis by EDS, the atomic concentration of $Cu_2O$ is 20%. Using low-voltage autoemission scanning electron microscopy it is shown that the microstructure of the initial Cu films strongly depends on the substrate temperature during condensation. This is attributed to condensation-stimulated diffusion. However, after atmospheric annealing, the differences between the samples smooth out. This is manifested in the decay of large crystallites of the sample deposited on the hot substrate. Due to this, the films of both series appear to be nanocrystalline with the most probable grain size of about 20 nm. It was shown that the effect of ammonia vapor on such films leads to a significant increase in their electrical resistance, which allows registering VOC. The resistance growth is accompanied by a change in the width of the band gap of semiconductors and the appearance of a low-energy optical absorption band. These effects occur at room temperature, i.e. the detector can operate without heating, which is mandatory in existing solutions. Relaxation of the detector is provided by its short-term UV irradiation, which returns the detector resistance and the energy state of semiconductors to the initial value. A model of chemical sensitivity that takes into account the nanocrystalline state of the films is proposed, and the prospect of using the detectors in technical applications is shown.

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# Artificial cuticle GREEN ARTICLE based on chitosan-hydroxyapatite bionanocomposite for poultry

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**Abstract ID #MTFC-1202**

The work improves the theoretical and applied aspects of the development of protective nanocoatings GREEN ARTICLE (ARTIficial CutiCLE) for poultry farming based on biomimetic approaches [1]. This technology is used in the production of table and hatching eggs from chickens, geese, ducks and turkeys [2]. A bird's egg shell is a multilayer bionanocomposite consisting mainly of calcium carbonate, the outer surface of which is covered with a thin layer of glycoproteins interspersed with nanosized hydroxyapatite balls Ca10(PO4)6(OH)2) [3]. The presence of a cuticle layer on the surface of food and hatching eggs prevents, first of all, the entry of harmful bacteria through the pores in the calcite layers of the shell through which gas exchange occurs between the embryo and the external environment. [4, 5]. In this case, GREEN ARTICLE protective nanocoating technology is used, which enhances the protection of eggs from harmful bacteria. It was previously shown that electrochemical and ultrasonic technologies for modifying a solution of chitosan in peroxide compounds (peracetic acid, hydrogen peroxide) with nanoparticles of oxides: titanium, iron, zinc and metals: titanium, copper, calcite make it possible to create protective coatings to extend the shelf life of table eggs and prevent contamination hatching eggs with pathogenic microflora, increasing the hatchability of eggs and the quality of chickens [1, 2].

In this study, nanospheres of hydroxyapatite Ca10(PO4)6(OH)2) were introduced into the chitosan matrix substance using electrochemical and ultrasonic treatment methods, which most closely imitated the biologically active and mechanical strength characteristics of natural cuticle. Thus, differences in the connectivity of nanospheres throughout cuticle layer may be associated with different rates of bacterial penetration among quail (2.22%), turkey (3.33%) and chicken (15.56%) [5]. It has been shown that in the storage technology for food eggs (chickens, geese, ducks and turkeys, the use of GREEN ARTICLE artificial cuticle based on chitosan-hydroxyapatite Ca10(PO4)6(OH)2) allows you to extend the period of transportation and storage of products by 38-45 days at a temperature of 24 °C, since it provides low gas and moisture permeability and high biocidal activity against pathogenic bacteria and viruses due to an increase in layer thickness to 6 -10 microns. In the case of GREEN ARTICLE based on chitosan-hydroxyapatite Ca10(PO4)6(OH)2) for hatching eggs (chickens, geese, ducks and turkeys} based on chitosan-hydroxyapatite, the technology reduces the degree of contamination of hatching eggs with pathogenic microflora by 99.13 - 99.20%, while simultaneously increasing the hatchability rate of eggs by 1.80% - 16.29% of the control, depending on the crosses poultry and storage conditions for hatching eggs.

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# A Comparative Assessment of Electrochemical Properties of Multifunctional Coatings $TiO_2$ and TiON for Biomedical Implant Applications

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**Abstract ID #MTFC-1211**

In the realm of implant applications, the corrosion resistance phenomenon against the intricate physiological environment within the human body is of utmost importance. Despite Ti64 alloy exhibiting commendable corrosion resistance along with good biocompatibility, it is vulnerable to corroding in complex biological environments, particularly for long-term applications [1]. Oxide multifunctional coatings serve as a resilient protective barrier against the corrosive environment, making them highly favored for implant coating applications [2]. In the present study, coatings of titanium oxide ($TiO_2$) and titanium oxynitride (TiON) were successfully developed on a Ti64 alloy substrate. Field emission scanning electron microscopy (FESEM) and Energy dispersive spectroscopy (EDX) were utilized to analyze the coating's morphology and elemental composition. The surface wettability of the coating was investigated by measuring the contact angle using the sessile drop method. The corrosion study was carried out using a potentiodynamic polarization test followed by electrochemical impedance spectroscopy (EIS) in the corrosive media of a physiological saline solution. The surface coated with $TiO_2$ and TiON showed higher wettability compared to the bare Ti64 alloy surface. Additionally, the wettability of the TiON coating was significantly better than that of the $TiO_2$ coating. The corrosion test results demonstrate that both $TiO_2$ and TiON coatings exhibited higher corrosion potential and lower current density values than bare Ti64 substrate. Whereas $TiO_2$ coating shows a higher polarization resistance than TiON coating as it forms a strong passivation layer due to its inert characteristics; conversely, the presence of nitrogen in TiON coating increases its electrical conductivity, leading to a higher corrosion rate [3]. Likewise, EIS results indicated that $TiO_2$ coating demonstrated better corrosion resistance compared to the TiON coating.

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# Hybrid Multilayered Heterostructures for Energy Applications Based on Easily Transferable Polydopamine Films

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**Abstract ID #MTFC-1261**

Until recently, polydopamine (PDA) was mainly applied as a surface initiator for several biomedical applications and as a "sticky" active component sensing platform. However, several previously overlooked properties of PDA, such as high mechanical response, have been coming to light as research on this material continues. Here, I will mainly focus on the role of PDA coatings in energy applications, such as their apparent universal role as photosensitizers and their behaviour when in contact with a semiconductor [1]. I will introduce some physicochemical aspects that make PDA an ideal coating for many photocatalytic applications, including results on various semiconducting materials and nanostructures [2]. Also, I will present some of the recent findings and theories on the origin of this behaviour, as well as some novel PDA architectures based on 2D-like PDA free-standing films and multilayered structures with exceptionally sharp interfaces and mechanical resilience [3].

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# Gaining Insights into Nitride Multilayer Deformation—an Atomic-Level View

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**Abstract ID #MTFC-1272**

Transition metal nitrides (TMN) have been widely applied in cutting-tool hard coatings due to their high hardness, good wear resistance, and high chemical stability [1,2]. Multilayer (ML) coatings consisting of individual nitride constituents can significantly improve fracture toughness and enhance the hardness of coatings, especially when they are constructed superlattice. The protective hard coatings are used in harsh environments, such as high temperatures and high loads, so understanding the coatings' deformation mechanism becomes critical. However, how the multilayer coatings are exactly deformed remains unclear, especially from the atomic–level [3,4].

Here, we show the deformation mechanism of single–crystalline and polycrystalline multilayers from the atomic level [3,4]. Previously, due to the lack of atomic resolution imaging, ML deformation is limited mainly to microscale observations. We found that slip and microcrack are the dominant deformation mechanisms in single–crystalline while grain boundary sliding is the primary deformation in polycrystalline multilayer. Except these, we found an entirely overlooked phenomenon occurring during the deformation of nanoscale multilayers, i.e., under nanoindentation, the multilayer structure is disrupted and forms solid solution zones [3], or creating high-density deformation twinning and stacking faults in some cases [5,6]. Our investigations demonstrate that the multilayer deformation exhibits variety from the atomic level, which could interpret distinct mechanical properties of various multilayers.

We anticipate that coupling advanced atomic-resolution characterization with the cross-sectional FIB cutting view on the deformed multilayers could reveal the ML deformation mechanism at the atomic level. This allows for correlating the microscale /atomic-scale structure with the macroscopic property of multilayers and will assist in understanding ML deformation during service conditions and designing the novel ML for applications. These observations also provide a valuable guide to metallic multilayers and the architecture of new heterogeneous materials.

## ACKNOWLEDGMENTS

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# Effect of Ferrocene Introduction on Electrical Properties of the $Bi_2Se_3$ Ultrathin Films

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**Abstract ID #MTFC-1319**

Topological insulators (TIs) are a new state of matter with an insulating bulk and topologically protected by time-reversal symmetry (TRS) gapless conductive surface states (SS). Breaking the TRS of TIs allows the opening of a gap at the Dirac point of topological SS, which offers the opportunity for different unique quantum physical phenomena to emerge (for example, quantum anomalous Hall effect [1]), which may have potential applications in the future spintronic devices. One of the effective approaches to breaking the TRS is the introduction of magnetic dopants into the TI crystal lattice [2].

In this work, the synthesis method to obtain ultrathin (up to 14 nm) ferrocene ($Fe(CH)_{10}$)-doped $Bi_2Se_3$ films on quartz substrates with different levels of iron doping is developed. To evaluate the influence of ferrocene introduction on the thermoelectric and electrical properties of the $Bi_2Se_3$ ultrathin films, the measurements of the thermoelectric properties of ferrocene-doped $Bi_2Se_3$ films were performed using a home-made system. The electrical properties of ferrocene-doped were performed at low temperatures down to 2 K using a physical property measurement system (PPMS).

The results showed that the charge carrier densities in ferrocene-doped $Bi_2Se_3$ films are lower in comparison with pristine films. This indicates that iron atoms substitute bismuth atoms and, thus, act as acceptors, which is the reason for the slight decrease in the charge carrier density [3]. Charge carrier mobilities of ferrocene-doped $Bi_2Se_3$ ultrathin films are distinctly reduced in comparison with the pristine films, which is related to an increased number of disorder levels in the $Bi_2Se_3$ crystal lattice due to the incorporation of iron atoms. Thermoelectrical properties of ferrocene-doped $Bi_2Se_3$ ultrathin films were investigated and compared with pristine $Bi_2Se_3$ films. The study of properties of ferrocene-doped $Bi_2Se_3$-based nanostructures helps to broaden the opportunities for the fabrication and utilization of thermoelectric and spintronic TI-based applications.

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# Advanced Functionalities in Polymer Composites through Embedded Smart Layers using Conductive Nanofillers

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**Abstract ID #MTFC-1328**

The integration of electrically conductive nanofillers such as multi-walled carbon nanotubes (MWCNTs), MXenes, and graphene into polymer composites has significantly enhanced their functionalities. The development of smart layers within polymer composites through the incorporation of those nanoparticles enables the creation of composites that not only retain their structural integrity but also possess advanced sensing and heating capabilities [1-4]. This review summarizes recent studies on the advanced properties imparted by these nanofillers, including crack propagation monitoring, strain sensing, Joule heating, and damage detection.

The strain-sensing capabilities of nanomodified composites with spray-coated MXene and poly(3,4-ethylenedioxythiophene) PEDOT-CNT have been particularly noteworthy. Three-point bending tests revealed that MXene coatings displayed a significant change in electrical resistance under tensile and compressive strains, confirming their high sensitivity and suitability for monitoring structural integrity [1, 2]. PEDOT-CNT coatings exhibited stable resistance changes under similar conditions, further demonstrating their potential for reliable strain sensing in flexible and dynamic environments. Both systems showed excellent sensitivity in a material's electrical resistance to strain with a gauge factor of 0.25-0.5. Furthermore, these coatings demonstrated uniform heating capabilities, reaching 50 °C in 120 s under a power density of 7.44 W, highlighting their potential for efficient Joule heating applications [1].

For damage detection, the use of MXenes and poly(acrylic acid) sodium salt PAANa-based coating has shown significant promise. The shape of equipotential voltage lines near the defect in the composite plate was precisely mimicking the geometry of the defect. It was possible to determine the location, quantification, and geometry of the damage by monitoring the voltage distribution throughout the spray-coated conductive layer [3]. Thus, showing the potential of providing real-time data on microcracks and other structural damages within the composite materials in practical applications.

Effective crack propagation monitoring was obtained with the introduction of MWCNTs spray-coated layer into glass fibre-reinforced plastics [4]. This capability was demonstrated in double-cantilever beam tests performed according to the ASTM D5528 standard, where the resistance change was correlated with crack growth, indicating the potential for real-time damage detection in structural applications [4]. Additionally, the correlation coefficient between the applied force for crack propagation and the electrical resistance was -0.945, indicating a very strong negative relationship between these two processes [4]. Thus, one of these processes can be controlled by the other and vice versa.

These smart layers show good potential in real-time damage detection, efficient heating, and precise strain sensing.

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# Degradation of Mechanical Properties in Layered Double Hydroxide-Modified Epoxy Coatings under Seawater Influence

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**Abstract ID #MTFC-1329**

Epoxy coatings are widely used for their excellent mechanical and protective properties. However, exposure to harsh environments such as seawater can significantly impact these properties. This study investigates the degradation of mechanical and sorption properties of CHS-Epoxy 582 coatings modified with Mg-Al/$NO_3$ layered double hydroxide (LDH) additives in seawater environments.

LDHs, characterized by their unique layered structure and intercalated nitrate anions, are known to enhance the barrier properties of coatings, reducing the penetration of corrosive elements [1, 2]. Four groups of epoxy films were prepared with LDH concentrations of 0, 1, 2, and 5 wt% and tested for mechanical properties and sorption behaviour. The chemical composition consisted of CHS-Epoxy 582, Telalit 0420 hardener, and LDH particles (supplied by SMALLMATEK, Aveiro, Portugal). Degradation tests were conducted in four different media: distilled water, seawater, 26 wt% concentrated salt solution at room temperature, and distilled water at 50 °C.

The results indicated that the diffusion coefficient of water in the epoxy matrix increased significantly with temperature, showing a 3-5 times rise in hot water compared to room temperature. The presence of salts in water increased the diffusion coefficient by up to 25 % in salt solutions. Equilibrium moisture content was influenced by salt concentration, with a higher salinity of 26 wt% reducing water absorption capacity by up to two times. Raised temperatures to 50 °C increased equilibrium moisture content by 20-30 %. Mechanical tensile tests revealed that LDH additives generally decreased mechanical properties such as elastic modulus and ultimate stress. At 5 wt% LDH, the elastic modulus decreased by 10-20 % for both aged and reference specimens.

Previous studies have used additional chemicals, solvents, and wetting agents to improve particle distribution. However, these additives often led to a significant decrease in the elastic modulus, sometimes by up to two times. This detrimental effect was not observed in specimens without any additives except for LDH. This study highlights the importance of optimizing chemical composition and processing conditions to balance the mechanical performance of epoxy coatings in corrosive environments.

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# Percolative 2D networks of Silver Nanowires. From Nanomaterial Large Scale Production to Real Life Application of Flexible Transparent Film Heaters

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**Abstract ID #MTFC-1333**

Transparent heaters (TH) have recently attracted intense focus from both academic and industrial researchers due to the key role they play in many technologies, including smart windows, deicers, defoggers, outdoor displays, actuators and sensors.[1] A new generation of THs based on nanomaterials has led to new paradigms in terms of applications and prospects in the past years.

We will present how silver nanowires appear as a real breakthrough in this field. When used in the form of random networks, they demonstrate remarkable performances for the fabrication of flexible THs, with excellent trade-off between sheet resistance (few Ω/sq) and optical transparency (>90%).

In this study, we measured the performances of various systems based on silver nanowires with independently controlled diameters and lengths, and performed a production scale-up, while taking care of the potential toxicity of the nanowires.[2]

We will present the fabrication of THs and their characterizations performed both at the nanoscale, in particular using lock-in thermography, and at the macroscale.[3] Several industrially driven applications using the flexible THs will also be presented and discussed.[4]

We will also show how silver nanowires can be assembled into 3D percolative networks in the form of aerogels.[5]

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# High-Entropy Alloys and Their Perspectives for Mitigation of Microbiologically Influenced Corrosion

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**Abstract ID #MTFC-1353**

High-Entropy Alloys (HEAs) and coatings represent a revolutionary class of materials defined by their unique equiatomic or near-equiatomic composition of multiple principal elements. This design philosophy unlocks a synergy of extraordinary mechanical, physical, and thermal properties stemming from the high entropy effect. This work delves into the fascinating world of HEAs, exploring their exceptional characteristics, including superior strength, hardness, and, crucially, corrosion resistance compared to conventional alloys [1-5].

The cornerstone of these outstanding properties lies in the formation of diverse atomic structures due to the high-entropy mix. This results in enhanced lattice stability and novel deformation mechanisms, paving the way for HEAs to excel in demanding environments. Furthermore, the inherent tunability of HEA microstructures allows for the creation of materials tailored for specific applications, from aerospace components to energy storage systems. This versatility positions HEAs as potential game-changers across various industries.

This research takes a bold step forward by exploring the design and development of HEAs with intrinsic antimicrobial properties. By harnessing their exceptional mechanical performance alongside the ability to inhibit microbial growth, HEAs offer a groundbreaking approach to mitigating Microbiologically Influenced Corrosion (MIC). This exciting avenue in materials science holds immense promise for developing innovative solutions in the fight against corrosion.

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# Improvement of Operational Properties of Power Equipment Parts Operating in a Loaded State

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**Abstract ID #MTFC-1358**

Coal-fired thermal power plants take a significant share in global electricity generation. According to the International Energy Agency (IEA), in 2022, the share of coal-fired power generation in global electricity generation amounted to about 36%. This indicates that the efficiency of thermal power plants has a significant impact on the productivity of most sectors of the economy.

The efficiency of high-temperature power plants is highly dependent on corrosion and erosion of particulate matter, especially at elevated temperatures. The cause and type of particulate corrosion and erosion varies from industry to industry and plant location, for example, particles may be fly ash in boilers, scaling in steam turbines, or minerals in oil production. [1; 2] Corrosion and erosive high-temperature wear of heat exchanger tubes and other structural components of coal-fired boilers has become a key problem in the design and operation of thermal power plants and is recognized as a major cause of downtime. [3]

Erosion and combined erosion-corrosion processes cause severe damage to equipment parts in various industries. Erosion and combined erosion-corrosion processes cause severe damage to equipment parts in various industries. These processes occur in a wide range of operating conditions applied to industrial parts, such as the operation of steam and water pipes, the operation of parts used in solid fuel preparation and combustion in the boiler furnace, the movement of steam and its impact on turbine blades [4]. The knowledge of such cases is necessary for the selection of suitable materials for the manufacture and design of parts operating in a loaded state. Common corrosion mechanisms are based on the mechanical effects of relative motion of gas or liquid (second body) and confined solid particles (third body), accompanied by oxidative and corrosive processes leading to increased wear. Thus, the exposed bulk surface is subject to chemical reactions with interacting oxidizing agents contained in the flowing liquid or gaseous medium.

The development of technologies for the application of protective coatings of boiler heating surfaces using thermal spraying, requires a careful assessment of the operational characteristics of the boiler. This evaluation should help to establish the influence of the boiler furnace characteristics on the properties of the protective coating.

Detonation spraying of coatings is one of the promising methods of applying a wide range of materials and movements with high velocities (more than 800 m/s) during the detonation spraying process, which results in negligible material degradation. In this way, dense coatings with excellent adhesion strength, low porosity and residual compressive stresses can be obtained. However, little information is available on the thermal expansion and recrystallization of such high temperature coatings. [5]

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# Effect of Artificial Intelligence on Obtaining Coatings and Materials with Specified Properties

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**Abstract ID #MTFC-1363**

The world's interest in exploring the moon and other planets of our galaxy requires all participants in these studies to develop and produce materials with given properties. The International Joint Institute of Advanced Coatings Technology of Taizhou University conducted research on the impact of artificial intelligence on the production of diamond-like carbon monocrystalline coatings with given properties. To obtain the desired coating with certain properties, we used knowledge of the relationship between the structure and the property of the bonds of carbon atoms, which needed to be included in the process of machine research. The use of a machine study of diamond-like carbon coatings allowed us to reduce the number of experiments by hundreds of times and generate the diamond-like carbon monocrystalline coating structure we need with given properties for the subsequent production of coating using PVD technology.

The effect of artificial intelligence on obtaining innovative functional coatings, obtained during our research, indicates significant prospects for the use of artificial intelligence in the production of coatings and materials with given properties.

P. Ying, Ch. Lin, P. Zhang, J. Wu, T. Yang, A. Kovalev, N. Myshkin, Vladimir Levchenko have additional affiliation - Zhejiang Provincial Key Laboratory for Cutting Tools, Taizhou University, Taizhou (China)

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# Developments in Indium Evaporation for Bump Bonding Applications

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**Abstract ID #MTFC-1369**

This presentation delves into the relationship between process parameters and indium evaporation for achieving optimal bump formation in advanced packaging. Parameters such as substrate temperature, deposition rate, crucible material, and evaporation geometry significantly influence indium film thickness, microstructure, and adhesion, which are critical for bump reliability and electrical performance. We will explore recent advancements in system engineering and evaporation techniques and their impact on bump uniformity and film morphology. By optimizing these process variables, this presentation aims to provide insights into enhancing the efficiency and effectiveness of indium bump bonding for next-generation electronic devices.

TRACK 5

# “NANOSCALE CHARACTERIZATION & IMAGING”

# Surface Stress Anisotropy of Silicon Reconstruction

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**Abstract ID #NCI-1032**

The unique reconstruction on the silicon surface is known to be based on dangling bond reduction and adatom formation. Although the rearrangement of the surface atoms largely reduces the electronic energy of the surface by reducing the number of surface dangling bonds, the surface reconstruction increases the surface stress and the surface energy as well. Among the silicon surfaces, a reconstructed Si(110)-"16×2" has a chiral structure (L or R) with one-dimensional mono-atomic steps and pentagon pair rows along [1-12] and/or [-112] directions. The chiral structure exists as a double domain on the surface, with the two combinations in equal proportions. It is known that the domain orientation on the surface is determined the direction of the monatomic steps pre-existing on the off-axis Si(110) plane, however, no method has yet been established to reproducibly and selectively control the homochirality on the on-axis Si (110) one.

Here we show the internal surface stress contrast between reconstructed Si(110)-"16×2" and hydrogen-terminated Si(110)-1×1 surfaces. We found the Si(110)-"16×2" reconstruction has anisotropic tensile stress intrinsically on the bulk Si(110)-1×1 structure. The anisotropic Si(110)-"16×2" structure has the potential to be tailored to self-assembled nanostructures by using uniaxial extrinsic stress. Furthermore, as expected, we were able to find selectively the chiral reconstructed structure. Our results demonstrate how to form homochirality on the Si surface, which consists of a one-dimensional chiral structure.

# Understanding the Cohesive and Adhesive Failures in Novel Multilayered SWCNT-Reinforced PDMS Composites Using Nano Scratch Technique

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**Abstract ID #NCI-1034**

Over the years, scholarly investigations have predominantly focused on elucidating the intricate mechanisms governing polymer wear, delineated into three principal classifications. Firstly, the two-term model has been extensively examined, explicating wear because of two primary phenomena: interfacial sliding (the adhesion component) and ploughing. Secondly, research has probed into the phenomenological drivers underlying wear mechanisms, encompassing abrasion, erosion, fretting, fatigue wear, chemical wear, and delamination wear. Lastly, attention has been directed towards discerning the nuanced variations in wear mechanisms exhibited across distinct classes of polymers, notably elastomers, thermosets, and thermoplastics [1-4].

This study focuses on investigating the nanoscale wear and failure of a synthetic elastomer-polydimethylsiloxane (PDMS). Nano scratch test is used as a nanoprobing technique on multilayered thin films made of neat PDMS and silane functionalized single-walled carbon nanotubes (Sily-SWCNT) reinforced PDMS composites to study the cohesive and adhesive failure in soft materials. Two types of novel layered composites are comparatively considered in this study: (i) LBL PNCs: Multilayered films with alternating layers of SWCNT and PDMS, and (ii) Bulk PNCs: Multilayered films with SWCNT reinforced in the bulk of PDMS matrix. Composites with four incremental concentrations of SWCNT at 0.05 wt%, 0.2 wt%, 0.5 wt%, and 1 wt% are comparatively studied.

Nano scratch tests (unidirectional single passes) are conducted using a Berkovich tip in a load-controlled mode in both single and ramp force conditions for a constant lateral displacement (scratch length) of 30 μm. The cohesive failure, which is a bulk property of the test structure, is correlated with the normal force used to initiate the scratch on soft films. Adhesive failure is the interfacial delamination of the film from the substrate. It is revealed as a breakpoint in the normal force vs normal displacement plot at the limit of the film thickness and is a measure of the interfacial strength of the film [3]. In LBL PNCs, the adhesive failure is used as an indicator of the interfacial adhesive strength between the SWCNT and PDMS. The coefficient of friction and scratch resistance are also calculated and correlated with the cohesive and adhesive energies. The structural properties of the test structures such as the film thickness, SWCNT network density, and 2D surface morphology of the top surface of the test structures are correlated with the resulting surface mechanical properties and failure modes obtained from the scratch tests.

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# Examining Stretch Marks in Soft Composites Using Field Emission Scanning Electron Microscope-Assisted In-Situ Nanoindentation Analysis

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In-situ Field Emission Scanning Electron Microscopy (FESEM) coupled with Nanoindentation analysis is primarily employed for visualizing deformation, crack propagation, and failure modes, while quantifying surface mechanics through force-displacement curves. While crack initiation and propagation provide crucial information on fracture mechanics in materials like metals, ceramics, and stiff polymers, visualizing cracks in highly elastic polymers such as polydimethylsiloxane (PDMS) poses challenges due to negligible permanent deformation at low nanoindentation forces. Consequently, fracture and failure, typically represented by cracks and delamination in such materials, manifest as partial to fully recoverable stretch marks. In-situ FESEM-assisted nanoindentation analysis emerges as a key technique for visualizing these stretch marks and correlating them with force maps.

This study focuses on silane functionalized single-walled carbon nanotubes (Sily-SWCNT) embedded PDMS composite (0.5 wt%) in a novel multilayered architecture with alternating layers of PDMS and SWCNT. Nanoscale plastic deformation and stretch marks on the top surface during deformation are reported by comparing stretch marks and force-displacement curves from nanoindentation analysis. The findings elucidate the impact of SWCNT reinforcement on nanoscale resistance to force flow along the top surface, observed in the resistance offered by the test structure against stretch mark propagation. Moreover, this nanoscale phenomenon is correlated with macroscopic delamination analysis to assess bonding strength across the composite's thickness.

The comparative examination of nanoscale and macroscopic deformations demonstrates that the incorporation of single-walled carbon nanotube (SWCNT) reinforcement in alternate layers enhances the resistance of the test structure to force propagation in both transverse and longitudinal orientations. This underscores the efficacy of the innovative multilayered design and its influence on enhancing mechanical integrity, particularly at low SWCNT concentrations within polydimethylsiloxane (PDMS). Such architectural configurations exhibit promising potential for application in lightweight, high-performance optoelectronic and electromechanical devices.

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# Nanoscale Characterization of Chalcogenide Thin Films for Memory and Energy Applications

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**Abstract ID #NCI-1095**

Chalcogenide materials possess distinctive material properties, making them promising candidates for a range of applications, including nonvolatile memory (e.g. neuromorphic computing) [1] and thermoelectric systems [2]. The microstructure of these alloys plays a crucial role in designing reliable devices. Understanding the local structure of different states and observing atomic scale changes are essential for optimizing device performance and comprehending the underlying transformation mechanisms. This talk discusses the nanoscale changes in Ge-Sb-Te (GST) thin films [3-5] and explores the local structure of Cu-Te thin films. These investigations are carried out via direct imaging in real space, utilizing analytical and in situ Cs-corrected scanning/ transmission electron microscopy (S/TEM).

The first part of the talk presents experimental findings on order-disorder transitions and interfacial transformations in GST phase change memory thin films. The control of disorder in these materials is vital for their applications, as the distribution of structural defects (vacancies) significantly impacts their physical properties. Structural transformations from vacancy disordered to layered vacancy-ordered and van der Waals-bonded GST structures are observed through in situ heating TEM. Detailed characterizations of GST grains unveiled transient structures, indicating shear transformation mechanism and different layered defects as well as chemical changes during transformations. Additionally, reversible self-assembled reconfiguration of structural order and the formation of novel structural GST units are observed during the exposure of atomic layers in GST to a focused electron beam. These results offer novel insights into phase formation and transformation mechanisms in GST systems, which are critical for refining their microstructure and hence their properties.

The second part of the talk delves into the controversial aspects of the local structure of layered Cu-Te. Here, various nanoscale Cu-Te phases are synthesized from $Cu/Sb_2Te_3$ thin films by thermal heating. Layered Cu-Te structures comprising double and triple layers of Te are found in the thin films. Contrary to existing literature, the favored double layered Cu-Te structure is determined as the trigonal $Cu_7Te_4$ phase, while the triple layered Cu-Te structure is identified as a new metastable Cu-Te phase. Because of its similarity to $Sb_2Te_3$, the new structure can be prepared through solid-phase epitaxy using magnetron sputtering at room temperature. These findings provide valuable insights into the local structure and preferred phases of Cu-Te that can be formed during the cycling of Cu-based thermoelectric materials [6], thereby paving the way for theoretical exploration of their properties and the design of new layered materials.

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# Exploring Nanostructural Behaviour of Xero- and Aerogels through Small Angle Neutron Scattering

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**Abstract ID #NCI-1106**

The open porous structure, large specific surface area, low density, low thermal conductivity, structural stability, and variable transparency render xerogels and aerogels suitable for diverse applications across industries, from pharmaceuticals and medicine to civil engineering and wastewater treatment. These sol-gel-derived materials exhibit significant variations based on synthesis procedures, functionalization, and structural fine-tuning. Small Angle Neutron Scattering (SANS), in conjunction with other techniques, plays a crucial role in characterizing their nano- and micro-level structures, elucidating the relationship between nanostructure and macroscopic properties. The contrast variation method employed in SANS enables the characterization of hybrid aerogel and xerogel materials, as well as the study of hydration mechanisms. Examples of SANS structural characterization include MTES/TEOS-based silica xerogels [1], vinyl-methyl-decorated silica aerogel-like hybrids [2], and contrast variation studies on borosilicate [3], calcium-alginate [4], and polyamide aerogels [5].

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# Thermostimulated Structural Evolution of Ge-Doped $HfO_2$ Nanolayers: Insights from Advanced Characterization Techniques

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**Abstract ID #NCI-1229**

The application of multicomponent materials necessitates comprehensive monitoring of their optical, luminescent, and electrical properties, supported by structural characterization and chemical composition analysis. Techniques such as X-ray diffraction, Raman scattering spectroscopy, and infrared reflection spectroscopy offer insights into morphology and crystalline structure, albeit with limited spatial resolution. Transmission electron microscopy provides detailed views of local crystalline structures, while scanning Auger microscopy offers high spatial resolution for analyzing elemental distribution in multicomponent nanoscaled materials.

In this study, we investigated the thermostimulated structural evolution of doped hafnia nanolayers deposited by radio-frequency magnetron sputtering on silicon substrates. Doping $HfO_2$ allows for modifying its structural properties for various applications, yet the impact of isovalent impurities like Ge and Si remains relatively underexplored. Our goal was to explore the structural properties of Ge-doped $HfO_2$ nanoscaled films, considering the effects of deposition conditions, Ge content, and annealing treatments.

The Ge concentration in the films ranged from 0 to 30 at %. Subsequent annealing treatments at temperatures ranging from 300 to 1100 °C for durations of 30 to 900 s in a nitrogen atmosphere were applied. Our results revealed that as-deposited films remained amorphous up to 600 °C, with phase separation occurring upon heating to 750-800 °C. This phase separation led to the formation of pure Ge nanocrystallites and tetragonal $HfO_2$ grains, with the temperature requirement varying based on the Ge content. Further temperature increase facilitated significant Ge out-diffusion from the films, resulting in the emergence of the monoclinic $HfO_2$ phase.

Importantly, no Si presence within the film volume or Ge segregation at the film/substrate interface was detected, indicating the stability of these films in direct contact with Si substrates. Through complex analysis using TEM and SAM methods, we discuss the mechanism of phase separation and compare our findings with previous research on Ge-doped $ZrO_2$ nanoscaled films, highlighting similarities and differences in structural evolution caused by the host nature.

# Positron Annihilation Lifetime Tools for Nanostructural Study of Spinel Ceramics

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**Abstract ID #NCI-1235**

The positron annihilation lifetime spectroscopy (PALS) method based on the fact that the unstable positron-electron system (positronium Ps) is repelled from ionic cores of atoms and tends to location in open pores. In the ground state, the Ps exists as singlet para-positronium p-Ps and triplet ortho-positronium o-Ps. In the case of ceramics, two channels of PALS should be considered – the positron trapping and o-Ps decaying. In general, these processes are independent ones. However, if trapping sites will appear in a vicinity of grain boundaries neighboring with free-volume pores, they can become mutually interconnected resulting in a significant complication of the measured PALS spectra. This occurs provided the input of one of the above annihilation channels will be significantly changed. To clarify this feature, we shall study the PALS characteristics of spinel-type $MgAl_2O_4$ ceramics affected to water sorption treatment enhancing o-Ps decaying over positron trapping modes.

The ceramic pellets were sintered in a special regime with maximal temperatures (Ts) of 1100, 1200, 1300 and 1400 °C during 2 h. The PAL measurements were performed with an ORTEC spectrometer ($^{22}Na$ source) placed between two sandwiched samples defpre and after water immersion. The obtained spectra were treated with LT computer program using four-component fitting procedure at high-statistical measurements.

The third and fourth components in the measured lifetime spectra are due to "pick-off" annihilation of o-Ps atoms in ceramics nanopores filled with adsorbed water. It is established that the $\tau_3$ lifetime increases with Ts, while its intensity $I_3$ decreases. These changes correspond to the increased nanopore size and smaller amount of nanopores. In all water-immersed samples, the intensity of third component $I_3$ significantly increases as compared with dried samples indicating a large content of absorbed water present in ceramics. This increase in I3 is accompanied by corresponding decrease in the first ($I_1$) and fourth ($I_4$) PALS components and increase in defect-related component ($I_2$).

The radius of free volumes where o-Ps are trapped in $MgAl_2O_4$ ceramics was calculated using the Tao-Eldrup model with character lifetimes $\tau_3$ and $\tau_4$. With increasing of ceramics sintering temperature Ts, the free volume radius $R_3$ increases from 3.09 to 3.31 Å and $R_4$ left nearly at the same level (~18 Å) in the samples taken after initial drying. In water-immersed samples, both nanopore radii $R_3$ and $R_4$ decrease with amount of adsorbed water, these changed being harmonized with nanopore content. In final, after ceramics drying, the initial state of these nanopores is partially restored. Thus, both types of inner nanopores in $MgAl_2O_4$ ceramics are practically identical in respect to efficiency of water sorption, but primary functionality of these ceramics is defined by smaller nanopores (defined by third PALS component) due to their prevailing content.

# Surface Modification by Low Energy Ion Beam

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**Abstract ID #NCI-1248**

Low-energy ion beam irradiation has emerged as a versatile technique with extensive applications in fields such as plasmonics, nanoelectronics, and nanomagnetism, etc. This method facilitates efficient large-scale fabrication of nanopatterns on diverse materials by precisely controlling ion parameters like incidence angle, energy, and fluence. Extensive studies have explored a wide range of morphologies including nano dots, ripples, triangular features, and holes on different materials with varying ion beam parameters [1-4].

This work investigates the formation of nanoripples and nanoterraces on soda-lime glass surfaces using ion beam irradiation, focusing on elucidating the underlying mechanisms. Our investigation systematically explores the impact of ion energy, fluence, and incidence angle on the structural morphology. Experimental findings reveal a distinct transition from ripples to terraces across a spectrum of ion beam parameters, spanning energies from 600 to 1500 eV and fluences between $9.7 \times 10^{17}$ to $2.0 \times 10^{19}$ ions/cm$^2$ at a fixed incidence angle of 45˚. The observed phenomena are elucidated through a modified Kuramoto-Sivashinsky (KS) equation [5], highlighting the critical role of non-linearity in terrace formation.

Moreover, the study showcases the tunability of glass surface wettability using ion beams, achieving desirable hydrophobic characteristics. The observed anisotropic hydrophobicity directly correlates with the amplification of nanopattern amplitudes on the surface, demonstrating the potential for tailored surface properties through precise pattern formation. This work significantly advances the fundamental understanding of ion beam-induced nanopattern formation while also emphasizing its practical applicability in surface engineering across various functionalities.

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# From Topography to Topology: The Use of Persistent Homology to Achieve a Deeper Characterization of Surface Nanostructures and Materials Properties

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**Abstract ID #NCI-1293**

In recent years, an algebraic topology method, named persistent homology (PH), has received attention from the community of materials scientists, due to the ability of the method to extract information from spatial structures [1, 2]. PH enables to study the multiscale connectivity of topological features of many materials science data, thus becoming a tool of materials informatics [3]. We present three case-studies to show the potential applications of the PH method to nanotechnology and surface science problems. One of the discussed examples regards the adhesion of magnetite nanoparticles, modified with a dopamine or polydopamine layer, to a gold surface. The relation between chemical composition, physical aggregation and adhesion properties is evidenced by analysis of the respective persistence diagrams (PD). The second case-study is related to electrodeposition of a metal-phenolic-network (MPN) layer on Indium-Tin Oxide electrode. The film growth mechanism is tracked ex-situ via atomic force microscopy (AFM) by a series of snapshots of the film morphology. In this case, PH is used to follow and characterize the dynamic evolution of the film morphology with increasing thickness of the MPN. Finally, the analysis of several nanostructured current collectors, to be used in anodeless batteries, is presented. Here, changes in process parameters lead to different nanostructures and we show how analysis of PDs is able to detect, classify and rationalize surface modifications.

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# Human Lung Cancer Tissue Morphology Analysis Using Atomic Force Microscopy

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**Abstract ID #NCI-1316**

As human lung cancer is a leading cause of cancer-related deaths worldwide, it's important to research it comprehensively. Various subtypes of lung cancer exist, each displaying distinct pathological and molecular characteristics, making it essential to study their morphological and molecular features [1]. Atomic Force Microscopy (AFM) is a powerful tool for studying biological materials such as lung cancer, offering high-resolution imaging at the nanoscale, and measuring tissue mechanical properties such as stiffness and elasticity, which are indicative of cancer progression. While AFM has been used to study various cancers, for example, human breast cancer biopsies [2], human liver cancer tissues [3], and even small human pulmonary arteries from tissue [4], AFM's application to human lung cancer tissues remains largely unexplored. This presents a promising yet underexplored opportunity to discover novel properties of different lung cancer subtypes.

In this study, we investigated the potential application of AFM methods in analysing human lung cancer tissue using histologically relevant biopsy preparation techniques. Human lung adenocarcinoma and squamous cell carcinoma tissue samples were prepared as tissue slices using cryosectioning and as single cell samples using liquid-based cytology. The tumour tissue sections were used for tissue and cell morphology imaging. Despite challenges arising from probe-sample adhesive forces, 5-10 µm thick tissue sections with scan areas from 2x2 to 60x60 $\mu m^2$ were examined using AFM tapping mode with scan speeds ranging from 0.17 to 1.35 Hz, achieving good image quality, and finding many micro-structured regions. Cytological – single cell samples were used for cell surface morphology and viscoelasticity studies, and measured in contact mode, successfully obtaining single cell images. Additionally, for AMF technique optimization different cell chemical fixation methods were compared using A549 cell culture and ASC52telo stem cell culture.

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# Femtosecond Holographic Microscopy: from Singe Nano-Objects to Magneto-Optical Imaging

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**Abstract ID #NCI-1336**

The development of femtosecond nanoscale imaging techniques with large fields of view has been hampered by the slow speeds of megapixel cameras, which make widefield imaging approaches prone to the accumulation of excess laser noise. Recently, we have combined off-axis holography with femtosecond pulses to overcome this longstanding issue and demonstrate shot-noise limited widefield ultrafast microscopy [1]. We have validated this technique by measuring the ultrafast response of dozens of single gold nanoparticles over a field of view of around 100 micrometers, demonstrating enough sensitivity to obtain transient images of gold nanoparticles down to 20 nm in diameter. Moreover, the holographic nature of this technique enables the reconstruction of the amplitude and the phase of the electric field, which can be combined with digital holographic refocusing techniques to localize nano-objects in three dimensions [2]. We demonstrated this by shooting 3D movies of the Brownian motion of dozens of 100-nm gold nanoparticles in aqueous solution in a 100x100x100 cubic micrometer volume of view.

The large fields-of-view enabled by the holographic imaging are also compatible with the study of ultrafast exciton and carrier diffusion properties. In typical experiments a single diffraction limited excitation spot is used, and the diffusion is tracked via the broadening of the transient signal around this initial spot [3]. Having a large field-of-view, we demonstrated how to create a pattern of diffraction limited, spatially separated excitation spots by imaging a pinhole array at the sample position. By doing so, one can perform exciton diffusion experiments around all excited spots spread throughout the image, which can be used either to address photophysical heterogeneity or to compute an average spot and vastly boost the sensitivity [4].

Finally, it is also possible to exploit the multiplexed holographic nature of the technique to encode polarization information. A traditional way to observe spin kinetics with femtosecond pulses is via time-resolved Faraday rotation, where spin-polarized states are generated using a circularly polarized pump, and the polarization rotation of a linearly polarized probe is measured using a Wollaston prism and a pair of balanced photodiodes [5]. This detection scheme automatically removes excess laser noise from the data, rendering it sensitive to small spin-related signals, but it does not have an equivalent in widefield microscopy. We show how polarization-encoding with off-axis holography solves this issue and demonstrate a widefield magneto-optical ultrafast microscope capable of simultaneously measuring the transient optical rotatory dispersion and the circular dichroism responses, which we validate imaging ultrafast spin kinetics in a lead halide perovskite.

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# X-Raying Just One Atom

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**Abstract ID #NCI-1341**

Since the discovery of X-rays by Roentgen in 1895, their utility has been ubiquitous, from medical and environmental applications to materials sciences. X-ray characterization of materials has been revolutionized after the invention of synchrotron X-rays in the mid-20th century. The capabilities of synchrotron light sources have been continuously upgraded, leading to the detection of an attogram amount of sample by X-rays. However, it is still in the range of $\geqslant 10^4$ atoms or more and further reducing the material quantity is a long-standing goal. This talk will present our recent groundbreaking X-ray spectroscopy and microscopy results of just one atom. Using synchrotron X-rays and a specialized detector tip positioned directly above a single atom in extreme proximity, X-ray excited current in a quantum tunneling regime can be recorded [1,2]. Using this method, a variety of X-ray spectroscopies, such as X-ray absorption spectroscopy (XAS), near-edge X-ray absorption fine structure (NEXAFS), and X-ray magnetic circular dichroism (XMCD), can be performed on just one atom. Thus, we can now simultaneously determine an atom's elemental, chemical, and magnetic properties on a one-atom-at-a-time basis. Moreover, we can now directly image individual atoms with chemical sensitivity using X-ray microscopy. These achievements open a new avenue of materials characterization, which will greatly impact many research areas from environmental, and biological to quantum information sciences.

## ACKNOWLEDGMENTS

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# Electron Microscopy of MXenes and Related 2D Materials

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**Abstract ID #NCI-1345**

MXenes are two-dimensional materials that have attracted substantial interest for applications in energy storage, electromagnetic interference shielding, catalysis, sensing, optoelectronics, medicine and many other fields.

The general formula for MXenes is Mn+1XnTz, where M is an early transition metal, X is carbon and/or nitrogen, and Tz represents surface terminations. [1] n indicates the number of parallel M layers in the 2D sheet and consequently gives an indication of the thickness of the material. Based on this general formula, it is apparent that the structure and chemistry can theoretically be varied to in excess of 100 different combinations. At present, more than 30 of these have been synthesized, including MXenes composed from a single transition metal, from solid solutions, as well as where different M elements are ordered in- and out-of plane.[2,3]

Characterization of these materials at the atomic scale is a prerequisite to understand the structure and to predict the properties using e.g. theoretical calculations. The tools that are commonly applied to investigate the MXenes constitute XPS and XRD, which measure the surface chemistry and separation of the parent material into individual sheets, respectively. However, to actually observe the structure of the MXenes at atpomic resolution require scanning transmission electron microscopy (STEM), equipped with EDX or EELS to explore composition and chemistry. [4]

Throughout the investigations of MXene, STEM has been employed to explore the structure of individual and multilayered MX sheets, including separation, stability and defects. STEM has further been used to explore the chemistry and stability of the surface terminations, Tz. [5] Through in situ methods, MXenes have also been exposed to different conditions, including high temperatures, gas, vapor and liquid inside the STEM.

In the present contribution, I will discuss and present some of the key findings about MXenes that have been gained through advanced electron microscopy and related methods. I will also present future directions on the characterization opportunities in the field of 2D materials.

## ACKNOWLEDGMENTS

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TRACK 6

# “NANOPHOTONICS”

# Quantum Cone as Source of Light with Dispersive Spectrum Radiation Distributed Along Cone Height and in Time

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**Abstract ID #NP-0915**

This work is devoted to developing a principally new nano source of light - a quantum cone. A quantum cone consists of many quantum dots with a gradually decreasing diameter from the base to the top of the cone. This distribution of quantum dots leads to a dispersive spectrum of radiation. Moreover, a change in the diameter of the dots leads to a change in the lifetime of excitons due to a change in the overlap of the Ψ functions of electrons and holes [1, 2]. The kinetics of photoluminescence from cones obey the stretch exponential law. This effect is explained by an increase in the excitons' lifetime along the cone's height from the top to the base of the cone. Moreover, there is an increasing concentration of excitons at the base of the cone due to their drift in the quasi-built-in electric field of the quantum cone [3]. The range of the dispersive spectrum depends on the material of the cone and its parameters [4]. The red edge of the spectrum is determined by the band gap of the bulk semiconductor and the blue edge by the quantum confinement of excitons on top of the cones. A quantum cone is a new type of nano source of light because it substitutes for two elements in a conventional spectrometer – a source of light and a dispersive element. These features of the quantum cone luminescence allow the construction of a spectrometer for measuring the absorption spectrum of individual nanoparticles or viruses.

## ACKNOWLEDGMENTS

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# Shift of Plasmon Resonance Peak: Effect of Magnetic Field Action

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**Abstract ID #NP-0989**

Surface plasmon resonance (SPR) is powerful method which allows very precise and accurate measurements of different type interactions happened on the surface of plasmon active metals (Au, Ag) in real time with ultra-high sensitivity. SPR has gained great popularity and represents a viable choice for many applications, from life sciences to pharmaceutics, agrifood and environmental monitoring of harmful substances [1]. Fundamental phenomena, which occurs at SPR detection are well-known and used to produce different high-quality sensors systems. But there is a number of features which take place when SPR observed and external magnetic field is applied at the same time. It means that the position of SPR-peak in transmittance spectrum (reflectance spectrum) is shifted due to action of magnetic field on the electrons motion influenced by the Lorentz force.

Optical properties of plasmon-polariton photodetectors [2] based on diffraction grating with period 630 nm were measured by spectroscopic ellipsometry (SE). The SE experiments were conducted at room temperature using the SE-2000 Semilab multi-angle spectroscopic ellipsometer (working wavelength range: 250–2100 nm, incidence angles were chosen 75º, 70º, 65º, 30º, 25º and 20º). From the SE measurements, the spectral dependencies of the ellipsometric angles $\Psi(\lambda)$ and $\Delta(\lambda)$ were obtained, from which the both real and imaginal parts of dielectric function was calculated using a optical model of the investigated material.

The influence of magnetic field action on and dependencies at different magnetic flux density (B=100-300 mT) and magnetic field direction: B ↑ ↑ n; B ↑ ↓ n; B ⊥ n (B and E are collinear), B ⊥ n (B and E are not collinear), where n – is normal vector to the sample's surface, for mentioned plasmon-polariton photodetectors were investigated. For B ↑ ↑ n and B ↑ ↓ n experimental configuration any changes in spectral dependencies did not exceed the measurement error up to an angle of 65° was reached. It was obtained, that magnetic field action results in both blue shift and altitude of characteristic SPR peaks of the structures under investigations. It was founded that in configuration B ⊥ n (B and E are collinear) noted effect was the most pronounced. For the certain experimental configuration B, n and E the effect was enhanced with a decrease of the angle of incidence, and for the smallest angle in our experiment (20°), it was most pronounced, which is in agreement with [3]. Possible physical mechanisms of observed phenomena are discussed. The results can open up new opportunities in the design of optoelectronic sensors of the magnetic field or high-speed optical modulators.

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# Sorption-luminescence method for determination of mefenamic acid

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**Abstract ID #NP-0995**

Sorption of the substance on the solid matrix is one of the effective methods to increase sensitivity and selectivity of luminescence (LM) determination. Luminescent chelates at low concentrations are not stable In solution, which limits their use in LM analysis of trace amounts of substances. Nanostructured materials that contain stable LM complexes of lanthanides (Ln) make it possible to significantly increase the LM quantum yield. However, during the synthesis of such phosphors the problems associated with the chelated Ln compounds encapsulation in the matrix often arise. The natural zeolites activated by Ln ions are such promising materials for solid-phase spectrofluorometry. These inorganic sorbents with crystal structures can include Ln ions in the grid using exchanged reactions. These ions save their ability to react with organic ligands. The sorbates that have been created on the zeolite surface can absorb UV-Vis-radiation and intensify LM. The possibility for mefenamic acid (MFA) [N-(2,3-Dimethylphenyl)anthranilic acid] LM determination using the Transcarpathian clinoptilolite (CL) as an efficient sorbent of Tb (III) was studied. MFA is a component of a common non-steroidal anti-inflammatory drug. The samples of CL-Tb(III) with a constant Ln content are obtained via Ln ions sorption from aqueous solutions at pH 8.25 on the CL in a solid phase extraction mode. The Cl-Tb(III) samples were precalcined at 250°C and treated with the alkaline water-ethanol solution, containing MFA. Obtained samples of the CL-Tb(III)-MFA luminophore were dried at 75°C. For the excitation of the LM samples rays with the λ=282nm are used. The LM intensity at 544 nm was chosen as the analytical parameter for the MFA quantitative determination. The proposed sorption-luminescent method allows to determine of MFA microgram amounts.

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# Investigation of Pulsed Mode Operation in Low-Temperature Arsenic Plasma Light Sources

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**Abstract ID #NP-1031**

Arsenic high-frequency electrodeless discharge lamps, used as photonic devices, have been previously explored for application in atomic absorption spectrometry (AAS) to detect arsenic in the environment at low concentrations. Such lamps are known for their stability and long lifespan, providing narrow spectral lines necessary for AAS [1]. Given that arsenic spectrum in the far UV region includes 3 resonance lines at 189.0 nm, 193.7 nm, and 197.3 nm, we have found that arsenic discharge lamps have potential applications in disinfection with similar or even better effectiveness than typically applied mercury-containing lamps [2]. However, under certain preparation and working conditions, arsenic lamps may begin to operate in a pulsed mode. The reasons for this phenomenon are still not fully understood. In this study, we investigate the behavior of arsenic lamps in the pulsed mode regime.

To create an inductively coupled plasma, spherical quartz bulbs with a diameter of 10 mm were filled with arsenic and argon at a pressure of 3 Torr. An outer electromagnetic field of around 100 MHz ignited the electrodeless discharge. The typical excitation voltage was set by a high-frequency generator within the range of 17-20 V. Emission spectra in dependence on time were recorded using a high-resolution spectrometer (Jobin Yvon SPEX 1000M) with a spectral resolution of 0.008 nm, coupled with a thermo-cooled CCD camera. The temperature fluctuations of the lamp during pulses were monitored using an infrared camera.

Our results showed that the repetition rate of pulses was higher for higher operation voltages. The temperature of As/Ar discharge was estimated to be about 950 – 1250 K. The temperature changes during pulses are in the range 250 – 400 °C. Our hypothesis of the observed phenomenon is that raising the temperature by higher operation power causes the increase of metal vapor pressure in the discharge volume. Consequently, electron collisions with element atoms, exciting and ionizing them, occur more frequently until, at some point, the electrons can no longer accumulate enough energy to continue these processes. Radial variation of temperature distribution was also detected.

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# Characteristics of Spectral Properties and Morphological Aspects in Thiacarbocyanine J-aggregates

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**Abstract ID #NP-1118**

Some organic luminophores can assemble into highly ordered molecular structures known as J-aggregates. These assemblies exhibit distinctive optical properties attributable to the excitonic nature (Frenkel-type) of electronic excitations. Described as low-dimensional molecular crystals, these aggregates are predominantly one-dimensional. In contrast to bulk crystals, the excitonic excitations within J-aggregates are localized within relatively small aggregate segments, termed exciton coherence lengths, rather than extending across the entirety of the aggregate. The dimensions of these segments are determined by the degree of disorder, whether energetic or topological, within the molecular aggregate. A hallmark of J-aggregate formation is the emergence of a novel narrow band, known as the J-band, which undergoes a bathochromic shift relative to the monomer band, typically coinciding with near-resonant fluorescence. Both the width of the J-band and the fluorescence lifetime are contingent upon the exciton coherence length: greater lengths result in narrower J-bands and shorter lifetimes.

The manifestation of excitonic excitations extends beyond the appearance of the J-band. Depending on the molecular arrangement within J-aggregates, an additional hypsochromically shifted band (referred to as the H-band) may emerge. The J-band arises from a "head to tail" molecular packing configuration, representing the lowest energy state of the exciton band, whereas the H-band arises from a "head to head" or "sandwich" molecular packing, representing the highest energy state of the exciton band, typically characterized by non-fluorescence. It is pertinent to note that the formation of H-dimers is a widespread phenomenon observed with various organic dyes. Certain dyes may concurrently exhibit both H- and J-bands in their spectra, leading to the designation of a "herringbone" structure. In such instances, their relative intensities and positions are contingent upon the molecular arrangement. The fluorescence of herringbone-type J-aggregates predominantly originates from the J-band.

The aggregation behavior of 3,3'-disulfobutyl-5,5'-dichlorothiacarbocyanine dye (TCC) in aqueous solutions underwent examination utilizing optical spectroscopy and microscopy techniques. Analysis revealed the predominant formation of dye H-dimers in water, with J-aggregation manifesting solely at elevated dye concentrations. Unlike conventional J-aggregates exhibiting "herringbone" structures, fluorescence spectroscopy unveiled the absence of optical interaction between H-dimers and J-aggregates. Fluorescent and electron microscopies unveiled fibril-like structures associated with the J-aggregates. Remarkably, for the first time, fibril disaggregation on spherical aggregates was observed under continuous electron beam illumination. The addition of NaCl or an acidic environment facilitated the shift of equilibrium towards J-aggregation, thereby enhancing aggregate spectral properties.

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# Upconverting Theranostic Nanoparticles Emitting in the UV to NIR Range

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**Abstract ID #NP-1186**

Cancer is one of the main causes of death worldwide; therefore, its accurate detection and efficient treatment is highly desirable. Theranostics is a medical field that combines diagnostic and therapeutic tools either simultaneously or sequentially [1-2]. Over the last two decades, lanthanide-doped inorganic upconverting nanoparticles (UCNPs) have attracted increasing interest in theranostics [3]. Such nanoparticles absorb two or more low-energy photons (usually in the near-infrared (NIR) range) and emit photons in the ultraviolet (UV) to visible (VIS) range. The emission spectra can be tuned by selecting appropriate lanthanide ion pairs, such as $Yb^{3+}/Er^{3+}$, $Yb^{3+}/Tm^{3+}$, and $Yb^{3+}/Ho^{3+}$. For application in theranostics, UCNPs should be small enough to penetrate cancer cells, thus offering localized effects. These UCNPs are also excited by (NIR) radiation, enabling deeper tissue penetration compared to UV or VIS radiation [4]. In addition, UCNPs typically exhibit a high signal-to-noise ratio, leading to high-contrast imaging [5]. However, for effective use in theranostics, UCNPs must emit light within specific spectral regions tailored to their intended applications. For example, emission in the red spectral region is crucial for photodynamic therapy, while UV or blue emission enables drug release, and NIR emission allows bioimaging using the NIR camera. Therefore, UCNPs that emit across multiple spectral regions offer both diagnostic and therapeutic capabilities within a single platform. Overall, these UCNPs hold promise for precise cancer diagnosis and treatment.

This presentation will detail the synthesis and post-synthesis treatment of upconverting core-shell-shell structured $NaGdF_4$:15%$Eu^{3+}$@$NaGdF_4$:49%$Yb^{3+}$,1%$Tm^{3+}$@$NaGdF_4$:5%$Yb^{3+}$,40%$Nd^{3+}$ NPs, emitting light from the UV to NIR range. Additionally, it will cover a comprehensive analysis of the structural and optical properties of the produced UCNPs, along with assessments of their colloidal stability (in aqueous and biological media) and biocompatibility.

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# Multicolor Luminescence of $NaGdF_4:Tb^{3+},Eu^{3+}$ Nanoparticles

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**Abstract ID #NP-1188**

Lanthanide-doped inorganic nanoparticles with unique multicolor luminescence (emission spectra containing multiple emission lines in different ranges of visible spectrum) are considered for many day-to-day applications (energetics, medicine, etc.) which means that the development of such materials is of high importance.

The goal of this study was to investigate luminescent characteristics of $NaGdF_4$ nanoparticles (NPs) co-doped with different molar ratios of $Tb^{3+}$ and $Eu^{3+}$. Therefore, a series of samples were synthesized via thermal coprecipitation method followed by detailed structural characterization of obtained NPs employing X-ray diffraction (XRD) and scanning electron microscopy (SEM) techniques as well as evaluation of their optical properties (excitation and emission spectra, decay curves) using Edinburgh Instruments FLS980 spectrometer.

XRD patterns of $NaGdF_4:Tb^{3+},Eu^{3+}$ samples confirmed hexagonal crystal structure of NPs synthesized. SEM images revealed that despite of different $[Tb^{3+}]:[Eu^{3+}]$ molar ratio the NPs of each sample have spherical shape and unimodal size distribution. After recording excitation spectra it was established that $NaGdF_4:Tb^{3+},Eu^{3+}$ NPs can be excited not only through $Tb^{3+}$ or $Eu^{3+}$, but also through $Gd^{3+}$. When NPs were excited through $Eu^{3+}$ ($\lambda_{ex}$ = 394 nm), all the samples emitted red light. If excitation occurred through $Gd^{3+}$ ($\lambda_{ex}$ = 272 nm) or $Tb^{3+}$ ($\lambda_{ex}$ = 368 nm), the overall emission color of NPs ranged from green to red which revealed the tunability of luminescence through manipulating $[Tb^{3+}]:[Eu^{3+}]$ molar ratio. In addition, decay curves of $NaGdF_4:Tb^{3+},Eu^{3+}$ samples provided photoluminescence lifetime values and allowed to evaluate $Tb^{3+} \rightarrow Eu^{3+}$ energy transfer efficiency.

According to our research, $NaGdF_4:Tb^{3+},Eu^{3+}$ NPs show plausibility as anticounterfeit pigments that would prevent various valuables (documents, money, medications, etc.) from being falsified.

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# Optical and Mechanical Properties of Polymer-Oxide - Carbon Nanotubes Composites

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**Abstract ID #NP-1201**

Micro/nanocomposites based on polymer (PMM/NC), e.g. cellulose, matrices are of wide applications due to their higher developed level, specific or sometimes unique properties and characteristics if compared to metal and ceramic composites. Thus, various types of PMM/NC containing dielectric nanoparticles have already been developed for specific applications. Polymers are widely used in industry and technology due to their easy production, light weight, and ductile nature as well. However, they possess some disadvantages such as low modulus and strength compared to metals and ceramics. That is why, the fillers (fibres, whiskers, particles) adding into polymer matrix is a way to enchance properties of polymers.

In this work we provide brief summary on morphology, structure and optical properties of the PMM/NC containing inorganic luminescent oxides providing composites to be attractive for modern optical devices. The features of the PL characteristics and the mechanisms of the PL excitation have been studied by us for the polymer matrixes filled with oxide phosphors of various spectral composition and decay. There were K2Eu(PO4)(WO4) (orange-red emission, fast decay), K3Tb(PO4) (green-yellow emission, slow decay), and SrAl2O4:Eu,Dy (green emission, long-lasting decay) in comparison with the PL characteristics of the specified phosphors in their "free" powder state. Carbon nanotubes (CNT) are the second filler of the composites under study. The CNT modify morphology, structure, mechanical, and electrical characteristics of composites, thus providing them with new properties. Correlations of the PL properties with morphology, spatial, electronic and vibrational structure of composites were identified and analyzed. The interactions between matrix and filler and their ability to determine the difference between optical properties of the noted hybrid composites and optical properties of matrix and filler are discussed in the work.

# Polymer Photonic Platform for Integrated and Quantum Photonics

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In the last couple of decades huge effort has been put into development of photonics platforms based on various materials such as Si, $Si_3N_4$, InP, $LiNbO_3$, GaAs and others. Only few of them (Si, $Si_3N_4$, InP) have turned into eco-systems resembling semiconductors industry of design house, foundries, fabless companies and multi project wafer (MPW) services of photonics integrated circuits (PICs). Silicon photonics is the dominant mostly due to compatibility with CMOS process. Silicon nitride photonics is gaining ground owing to the broad wavelength range starting from visible wavelengths allowing applications also in biophotonics among tele/Datacom and optical signal processing [1]. InP allow possibility to implement both active and passive devices on a single chip [2]. While various photonic platforms have matured to industrial level, they still have numerous challenges including limits set by material properties, expensive fabrication and complicated hybrid integration.

Polymer materials provide numerous advantages over semiconductor and oxide/nitride platforms: combination of passive and active elements, simple fabrication techniques mostly by spin coting, integration of other elements for hybrid platform, visible and near infrared wavelength range and multilayer structure [3]. As an additional advantage, the emission and non-linear optical efficiency of organic materials should be mentioned, which is many times higher than inorganic materials.

The thin polymer films are prepared by the method and applied to a glass or quartz glass substrate. This is one of the advantages, because there is no need for silicon or any other specific material wafers. In fact, it could also be applied on a flexible surface. The structure is recorded using the lithography method. Laser direct recording lithography is used to record microstructures and optimize the process. Next, it is possible to use parallel beam recording to speed up the process. Electron beam lithography is used to record nanostructures such as Bragg gratings. The fabricated structures are evaluated by optical and electron beam microscope. For resonators, the Q-factor was evaluated, and for light couplers, the optical losses in the waveguide.

During the development of polymer photonic platform we have established the workflows for the fabrication of passive elements (waveguides, power splitter, directional couplers etc) and active elements (discs, rings etc) mainly based on SU-8 and polymethylmethacrylate photoresist. The benefits of polymer photonics platform in respect to the already existing platforms, its possible application in quantum integrated photonics and our achievements in developing polymer photonic platform will be presented.

## ACKNOWLEDGMENTS

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# Plasmon-Exciton Polaritonics for Optical Sensing Applications

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Recently, there has been an enormous attention in the study of strong coupling between plasmon active metal nanostructures and various multi-emitters such as excitons in semiconductors, in organic dyes or photochromic molecules in complex photonic circuits. Photonic nanostructures which are able to support energy exchanges in strong coupling regimes have emerged as an exciting platform for manipulating light-matter interaction at the nanoscale [1], ultra-sensitive optical biosensors [2]. The main feature of strong coupling regime is that the energy exchange between the plasmons and the emitters occurs during a coherent time. This combines the desirable properties of nanophotonics and plasmonics: electromagnetic field enhancement which extended over large volumes with long-range order condensate optical states. Special attention will be paid for the reduction of losses in the hybrid plasmonic modes [3], its propagation length and extended coherence properties. The examples of employing hybrid plasmonic modes, plasmon-labelled protein polaritons formation for the biosensing applications [4] in detection of proteins interactions will be presented. Potential applications of strongly coupled plasmonics based nanostructures for the suppression of photobleaching by plasmon polaritons which successfully demonstrated in Fluorescence Life Time Microscopy (FLIM), also new type of the coherent light sources will be discussed.

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TRACK 7

# “TRANSPORT PROPERTIES IN NANOSCALE SYSTEMS”

# Swelling Behaviors of Alginate-based Composite Hydrogels Filled with Layered Nanoclays

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The Polysaccharide-based hydrogels (HG) are hydrophilic, insoluble cross-linked polymers that can absorb and retain large volumes of aqueous solution within their three-dimensional structure. Such hydrogels have many applications in various fields, such as biomedicine, pharmacy, cosmetology, food industry, water purification and agriculture. HG have a number of advantages, the most important of which are high biocompatibility, biodegradability, nontoxicity, and the ability to stimulate tissue regeneration. Some of the most well-known polysaccharides used to create HG are alginate, pectin, chitosan, hyaluronic acid, gum arabic, xylan, cellulose and their derivatives. Each polysaccharide has its own unique properties and functions that can be tailored by modifying its structure or combining it with other components, or nanoparticles.

The work focused on the study of composite HGs consisting of natural polysaccharide sodium alginate (SA) filled with the nanoclays montmorillonite (MMT) and LaponiteRD (Lap). SA is a biocompatible, biodegradable and gelling polymer derived from brown algae. MMT is a clay mineral with high surface activity, cation exchange and adsorption capacity, and Lap is a synthetic clay that is characterized by nano-sized anisotropic primary particles with a thickness of 1 nm and 25 nm in diameter. A series of composite SA based HGs with different nanoclay filler content were synthesized by ionic cross-linking with $CaCl_2$ aqueous solution. The structure of the synthesized HGs was characterized using SEM and FTIR methods. The main patterns of swelling of the synthesized HGs were determined and it was shown that swelling degree (Q) decreases with increasing concentrations of cross-linking agent and filler. The concentration of the crosslinking agent in the range of 0.3-0.5 wt.% $CaCl_2$ was chosen as optimal for synthesis of mechanically strong hydrogels with a high swelling degree. The maximum degree of swelling for HGs with MMT reached to 66.2 g/g, and for HGs with Lap it was 77.6 g/g at filler content of 20 wt.% and 0.3 wt.% $CaCl_2$. Classical equation (1) were used for characterization of water diffusion type during HGs swelling [1]:

$$F = Q_t/Q_e = kt^n \quad (1)$$

The values of $n$ and regression coefficients were calculated from the slopes and the intercepts of the plots of ln$F$ vs ln$t$. The Fick's diffusion transport is defined by $n$ and this value is used for determining the diffusion type. The calculated swelling exponent values ($n$) are close to 1 at 0.25 wt.% of $CaCl_2$ and 0.61-0.99 at 0.3-1 wt.% of $CaCl_2$ and 0.32-0.67 at 2 wt.% of $CaCl_2$. These swelling exponent values indicate < 0.5 Fickian transport; at 0.5–1.0 an anomalous non-Fickian transport included a mixed mechanism of diffusion and chain relaxation and values of n greater than 1 reflects the so-called Super Case II transport. The values $R^2$ varied between 0.97–0.99 for all HG.

## ACKNOWLEDGMENTS

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# A Mesoscale Model for the Diffusion of Nanoparticles in Biological Fluids: the Challenge of the Protein Corona

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**Abstract ID #TPNS-0998**

Nanoparticles (NPs) hold great promise in various medical applications, serving as targeted drug delivery vehicles and advanced diagnostic probes. However, their efficacy heavily relies on their ability to navigate the crowded biological environments within living organisms. In these environments, NPs encounter a polydisperse mixture of biomolecules at high volume fractions, which can hinder their mobility, leading to reduced diffusion. Understanding the mechanisms governing NP diffusion in such environments is crucial for designing more efficient materials for nanomedicine applications and predicting their toxicological effects.

This project proposes a computational approach to investigate NP diffusion in crowded environments. We develop mesoscale models that effectively mimic NP diffusion in biological fluids. Existing computational models and scaling theories on macromolecular diffusion often fail to account for the combined impacts of the Protein Corona (PC) and the crowded medium on NP behavior. By addressing the interaction of nanomaterials with protein-rich environments and considering both explicitly and implicitly the PC, this study aims to significantly improve our understanding of NP behavior. Findings indicate that corona morphology and polydispersity minimally affect diffusion, while introducing a novel descriptor crucial for understanding NP mobility. Additionally, our results suggest that the equivalent Stokes sphere approximation of the NP-PC results in a poor estimation of the diffusivity, and a different approach for the equivalent single sphere representation is here proposed. This simplification would enable hydrodynamic interactions to be calculated in a computationally tractable manner in future studies. Overall, this research contributes to advancing our understanding of NP behavior in biological fluids, offering insights for nanomedicine and nanotoxicology applications.

## ACKNOWLEDGMENTS

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# Surface Capping Layer Materials For 3D Topological Insulators

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**Abstract ID #TPNS-1011**

Bismuth selenide ($Bi_2Se_3$) is classified as a 3D Topological Insulator (TI), notable for its insulating bulk and conductive surface states, similar to those found in graphene. For harnessing nontrivial properties of the topological surface states towards the development of future nanoelectronic devices, it is crucial to preserve the surfaces of TIs as they tend to rapidly oxidize in the atmosphere. Engineering of an appropriate surface capping layer is one possible solution for minimizing the impact of surface degradation on charge carrier transport characteristics of 3D TIs, ultimately avoiding undesirable band bending effects that lead to the formation of two-dimensional electron gas (2DEG).

In this study, we explore the impact of several nanometres of surface capping layers fabricated using atomic layer deposition (ALD) technique for thin $Bi_2Se_3$ flakes, exfoliated from monocrystal. Our examination of charge transport properties of $Bi_2Se_3$ capped with several nanometres of zinc oxide (ZnO) uncovered notable changes in electronic behavior. This investigation provides characteristics of improved 3D TI materials and pinpointing the essential fabrication parameters for preserving topological surfaces allows further fundamental studies of topological surface states.

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# Electronic Properties of CVD Grown 2D $WTe_2$ on h-BN Surfaces

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$WTe_2$ is one of transition metal dichalcogenides possessing variety of exotic electronic properties, such as Type-II Weyl semimetal phase in bulk and two-dimensional topological insulator characteristics in monolayer materials. It exhibits also a large, non-saturating magnetoresistance, making it promising for applications in sensors and memory devices [1]. For fundamental studies of topological insulator and semimetal phenomenology towards new electronic devices employing topologically protected charge transport, development of reliable and scalable synthesis method for $WTe_2$ on insulating substrates is crucial. So far first experimental studies of exotic electronic properties of $WTe_2$ have been accessed in heterostructures with hexagonal boron nitride (h-BN). Here h-BN stands out as one of the best substrate materials due to its 2D nature, superior insulating properties, and high crystallinity. $WTe_2$/h-BN heterostructures are typically obtained by exfoliating and stacking of h-BN and $WTe_2$ on flat substrates. This approach allows to produce high-quality devices but is lacking scalability and fabricated structures are challenging to reproduce. Therefore, alternative methods for obtaining 2D $WTe_2$ on h-BN surfaces are necessity.

In this study, we have investigated CVD synthesis methods for obtaining $WTe_2$/h-BN heterostructures on insulating substrates ($Si/SiO_2$ and $Si/SiO_2$/h-BN). By adjusting determined CVD parameters of 2D $WTe_2$ structure growth on $Si/SiO_2$, $WTe_2$ was successfully synthesized on both h-BN monolayers and exfoliated h-BN flakes. Fabricated $WTe_2$/h-BN heterostructures were investigated using Raman spectroscopy and X-ray photoelectron spectroscopy (XPS). Moreover, CVD grown 2D $WTe_2$/h-BN heterostructures were then encapsulated to protect from rapid surface oxidation and used for studies of electronic properties via magnetotransport.

Our developed CVD growth protocols allow to fabricate $WTe_2$/h-BN reproducibly and determined charge transport characteristics of mono- and few layer CVD grown $WTe_2$ on h-BN confirm high-quality materials, suitable for further fundamental studies.

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# Magnetoresitance of an Array of Iron-Filled Aligned Carbon Nanotubes

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**Abstract ID #TPNS-1123**

The work presents the results of studies of magnetoresistance in an array of aligned multiwalled carbon nanotubes (MWCNTs) filled by iron. The array of aligned MWCNTs has been grown on a silicon substrate by the CVD method using ferrocene as an iron source. As the structural studies have shown, each MWCNT of array contains in the inner cavity several iron particles with a diameter of up to 10 nm. Atomic planes in the particles located in the inner cavity of the CNT are not oriented parallel to the axis of the CNT and form an angle with it.

The magnetoresistance of the array of aligned MWCNTs has been measured with two different current directions through the sample. In the first case, the current was directed along the axis of the CNT, the voltage drop was measured along the length of the tube. In the second case, the current through the sample has been directed perpendicular to the axis of the tubes. For each of the two current directions through the sample, the angular dependences of the magnetoresistance have been obtained. The angle between the direction of the current and the direction of the magnetic field through the sample was 0° (longitudinal magnetoresistance), 30°, 60° and 90° (transverse magnetoresistance). The studies of magnetoresistance have been carried in the temperature interval (77 – 293) K and magnetic field up to 2 T.

Studies have revealed some features in the resistivity and magnetoresistance of the array of filed with iron MWCNTs. The resistance of an array of MWCNTs in the direction along the axis of the tubes in a zero magnetic field is $5 \cdot 10^{-6}$ Ohm·m, and this value is three orders of magnitude lower than the resistance of an array MWCNTs in the direction perpendicular to the nanotube's axis. The magnitude of the magnetoresistance and the character of its field dependence significantly depend on the direction of the current through the sample and the orientation of the sample relative to the magnetic field. Thus, for example, the magnetoresistance perpendicular to the nanotubes axis does not exceed 2%, while the magnetoresistance in the direction of the tubes axis ranges from 30% for the longitudinal magnetoresistance to 100% at an angle of 60° between the direction of the current and the direction of the magnetic field through the sample. For a transverse magnetoresistance and at an angle of 60° between the direction of the current and the magnetic field through the sample, saturation in the field dependence of the magnetoresistance is not observed, while for a longitudinal magnetoresistance and at an angle of 30° between the direction of the current through the sample and the direction of the magnetic field, the saturation in the field dependence of the magnetoresistance has place already at a magnetic field of 0.5T.

The obtained in work results are analyzed in the terms of the giant magnetoresistance effect.

# Influence of the Insulator on the Electrical Properties of Discontinuous Iron-Insulator Multilayers

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**Abstract ID #TPNS-1149**

Metal-insulator granular films are a type of nanostructured material that consisting of metal nanoparticles embedded in an insulator matrix. Intensive research has focused on optimising their composition and structure to tailor their magnetic and magnetotransport properties. The control of magnetic parameters and magnetoresistance (MR) enables the development of advanced magnetic sensors, magnetoelectronic logic or spintronic devices [1, 2]. One of the key issues for a better understanding and control over of MR is the study of the electrical properties of metal-insulator granular films, namely, the temperature effect on the electrical resistivity.The aim of this work is to investigate the influence of the insulator matrix on the electrical properties of $[Fe/I]_n/S$ discontinuous multilayers, where I = $SiO_2$, MgO or $HfO_2$.

Magnetron sputtering was used for the deposition of $[Fe(d_{Fe})/I(3)]_{10}/S$ discontinuous multilayers, where $d_{Fe}$ = 2-7 nm. The substrate temperature was room temperature and remained unchanged during the condensation process. The deposited films were annealed to different temperatures (200 and 400 °C) in an Ar+$N_2$(2%) environment using an annealing furnace with a continuous gas flow. The crystal structure of thin films was analyze by the Transmission Electron Microscope JEOL 2100F UHR.

The resistivity ($\rho$) of the samples after deposition and annealing at different temperatures decreases with increasing effective thickness of the metal layers, regardless of the type of insulator layers. For as-deposited systems, the minimum value of $\rho = (5\text{-}10)\cdot10^{-7}$ Ω-m is fixed at the maximum thickness of the Fe layers. For samples annealed at 400 °C the resistivity reaches maximum values of 0.05-0.1 Ω-m at $d_{Fe}$ = 2 nm. Relatively high values of $\rho$ can be explained mainly by the formation of oxide phases. For layered structures with different types of dielectric layers and different thicknesses of Fe layers, the analysis of the temperature dependence of the resistivity (in the range of 20-300 °C) showed that (i) At dFe layers = 2 nm, the exponential nature of the $\rho$(T) dependence is observed for all structures, regardless of the type of insulator layers. (ii) At $d_{Fe}$ = 7 nm the exponential nature of the $\rho$(T) dependence is observed only for structures with $HfO_2$ insulator layers. Metallic temperature dependence of the resistivity is observed for structures with MgO and $SiO_2$ insulator layers; (iii) The transition from exponential to metallic temperature dependence of the resisitivity occurs at $d_{Fe}$ = 4-5 nm. This type of conductivity is determined both by the conductivity along the percolation cluster and by tunnelling between individual metal clusters that were not part of the percolation cluster.

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# Transport Phenomena During Nanofluids Flow in Channels in the Laminar-turbulent Transition Region

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**Abstract ID #TPNS-1158**

Nanofluids (NFs) are considered promising heat transfer carriers for refrigeration and heat power systems. Nanoparticles (NPs) in liquids significantly affect their thermophysical properties. Moreover, the presence of the NPs in the liquid contributes to the increase in both pressure loss and heat transfer coefficients during liquid flow, which cannot be explained by only variation in the nanofluids' thermophysical properties. For today, the effect of NPs concentration in liquids on the critical Reynolds number corresponding to the laminar-turbulent transition has not been examined adequately. Here we demonstrate that there are contradictory experimental results in published studies on the effect of NPs concentration on the critical Reynolds number corresponding to the laminar-turbulent transition during the liquids flow in channels. There are a number of studies that have experimentally confirmed the acceleration of the laminar-turbulent transition for various nanofluids with NPs mass fraction increasing. At the same time, there are studies where the laminar-turbulent transition is unchanged or even retarded. In the presented study, the own experimental data (nanofluid tetralin+$C_{60}$ up to 0.655 mass% and nanofluid isopropanol+$Al_2O_3$ up to 4.71 mass%) analyses, which show a decrease in the critical Reynolds number vs. NPs concentration increase. Various hypotheses of the effect of the NPs in the flow liquid on the variation of the critical Reynolds number are discussed. The obtained results will contribute to improving the understanding of the momentum and heat transport phenomena in nanofluids.

# Magnetotransport Properties of CNT/$Bi_2Se_3$ Heterostructures with an Enhanced Seebeck Coefficient

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**Abstract ID #TPNS-1324**

Thermoelectric materials and devices based on them, providing direct heat-to-electricity conversion, are an attractive solution for increasing the energy efficiency of domestic and industrial processes by capturing waste heat and converting it into useful energy. One of the main strategies for improving the thermoelectrical efficiency of such devices is the use of heterostructures containing materials with a high Seebeck coefficient, and high electrical but low thermal conductivity. A network of CNTs combined with nanostructured thermoelectric material such as $Bi_2Se_3$ provides an interface for efficient phonon scattering, resulting in reduced lattice thermal conductivity in heterostructure and promoting an effective charge transfer between these compounds. This may result in a significant improvement of the thermoelectric properties of the CNT/$Bi_2Se_3$ heterostructures.

Here, we demonstrate the synthesis of *p*- and *n*-type doped CNTs with its different weight amounts (wt.%) in heterostructures with $Bi_2Se_3$ nanostructures. Magnetoresistance measurements as a function of temperature of both individual compounds and heterostructures based on them were carried out in the temperature range from 300 to 2 K to distinguish the influence of different conducting channels and to identify mechanisms that determine thermoelectric properties of $Bi_2Se_3$/CNT networks. Magnetoresistance of pure CNT networks exhibits a semiconducting behavior (resistance increase towards lower temperatures), whereas the $Bi_2Se_3$ film demonstrates a metallic behavior (resistance decrease towards lower temperatures). A decrease in the wt.% of CNTs in the $Bi_2Se_3$/CNT heterostructures led to a change in the dominant mechanism in the overall conductivity (the transition from semiconducting (CNT-dominated) to metallic ($Bi_2Se_3$-dominated) behavior). The $Bi_2Se_3$/CNT heterostructures with the minimum possible amount of CNTs exhibit a higher Seebeck coefficient than individual components. This is a sign of the action of an additional electrical/thermal transport channel formed at the interface, which results in improved thermoelectric properties.

Magnetoresistance as a function of magnetic field for all obtained samples was measured up to 9 T. It can be concluded that the total conductivity of $Bi_2Se_3$/CNT heterostructures is determined by the CNTs component, and with an increase of wt.% of CNTs their influence increases. In addition to the dominant behavior of CNTs in conductivity, a strong WAL effect was observed in the temperature range of 2-10 K. This is a clear indication of the influence of the topological material.

Thus, the best networks for thermoelectric applications should consist of as small as possible amount of *n*-CNTs, covered with a thick enough $Bi_2Se_3$ layer to make continuous coatings and robust interface with CNTs. These findings illustrate the high potential of the CNT/$Bi_2Se_3$ heterostructures for applications in different heat-to-electricity conversion devices.

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TRACK 8

# “NANOMAGNETISM & MAGNETIC MATERIALS”

# Yttrium-iron Ferrite Garnets: Structural and Magnetic Properties vs Precipitation Route

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Magnetic materials based on yttrium-iron ferrites $Y_3Fe_5O_{12}$ (YIG) with the garnet structure are of significant attention for developing devices for modern communication systems and radiolocation. The key advantages of such materials include high magnetization values, specific electric resistance, and low energy losses. Usually, the electrophysical parameters of YIG-based materials are sensitive to their chemical composition, microstructure, and synthesis conditions. They can be tuned for the defined real-life purposes by partial substitutions in the cationic sublattices. For instance, YIG garnets with aluminum doping in iron sublattice are characterized by low magnetic and dielectric losses and increased dielectric constant that is crucial for a number of microwave devices [1]. The most common ways to fabricate YIG-based materials are solid-state reactions method and sol-gel technology. However, neither of them ensures sufficient level of quality of resulting material: garnets obtained via solid-state reactions have low chemical homogeneity due to the mechanical mixing of the starting reagents when garnets prepared via the sol-gel route cannot be easily washed away from the side products, which may negatively affect the electrophysical parameters of the following calcinated samples.

The main objective of this research was to synthesize Al-doped $Y_3Fe_5O_{12}$ garnets via precipitation in aqueous solutions and assess how the sequence of metal cations precipitation affects the magnetic parameters of resulting ferrite garnet samples.

A set of $Y_3AlFe_5O_{12}$ garnet particles was synthesized by the precipitation in aqueous solution at constant pH, varying the sequence of precipitation of metal cations. The coefficient of filtration for precipitates was determined, and collected data pointed that the best filtration ability was observed for precipitate obtained via the following route: $Fe(OH)_3$ and $Al(OH)_3$ were precipitated at pH 4 ÷ 4.5 and $Y(OH)_3$ – at pH 8.8 ÷ 8.9. DLS data allowed connecting this experimental observation with the micelle formation occurring during the precipitation processes. XRD and magnetic measurements for YIG powders obtained at 800°C revealed the dependence between the sequence of precipitation of metal cations and coefficient of filtration, formation of the crystalline structure, and magnetic parameters (saturation magnetization, coercive force).

All the sets of the synthesized $Y_3AlFe_5O_{12}$ powders were used to fabricate the ceramics. The effect of the variation of technological conditions during the synthesis of the powders on the magnetic parameters of corresponding ceramic samples was studied and analyzed. The obtained knowledge is essential for the optimization and simplification of the technology for large-scale fabrication of YIG-based materials promising for real-life practical applications.

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# Effect of Light Element Diffusion Through Artificial Grain Boundaries in Microfabricated Sm(Fe-Co)-B Dot Arrays

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**Abstract ID #NMM-0956**

$RFe_{12}$ (R: Rare-earth elements) compounds with $ThMn_{12}$-type structure have been considered as promising candidates for next generation permanent magnet materials because of their excellent saturation magnetization and anisotropic magnetic field with a minimum usage of rare earth elements. Recently, it has been reported that an epitaxial $Sm(Fe_{0.8}Co_{0.2})_{12}$ thin films has excellent magnetic properties such as saturation magnetization $\mu_0 M_s$ of 1.78 T, anisotropic field $\mu_0 H_a$ of 12 T and Curie temperature $T_C$ of 859 K [1]. Subsequently, it was confirmed that by adding B to the $Sm(Fe_{0.8}Co_{0.2})_{12}$ thin film, an anisotropic columnar structure was formed and a large coercive force $\mu_0 H_c$ of 1.20 T was achieved [2]. However, the $\mu_0 H_c$ of the obtained $Sm(Fe_{0.8}Co_{0.2})_{12}$-B thin film is only 10 % of $\mu_0 H_a$ = 12 T. On the other hand, it has been reported that the $\mu_0 H_c$ of Nd-Fe-B thin film increased from 0.98 T to 1.28 T by isolating the magnetic coupling between the main phases of Nd-Fe-B thin film through micro-fabrication of square dot arrays [3]. Therefore, the micro-fabrication method is considered to be one of the candidates for improving and elucidating the mechanism of coercivity.

In this study, to increase the coercivity of $Sm(Fe_{0.8}Co_{0.2})_{12}$-B thin films, micro-fabricated films were prepared, and various light element cap layers were deposited on the square arrays. Then, the samples were post annealed with various annealing temperature and crystal structure, magnetic properties and surface profiles have been investigated. $Sm(Fe_{0.8}Co_{0.2})_{12}$-B thin film were prepared using an ultra-high vacuum (UHV) magnetron sputtering system. The film structure is V (20 nm) / $Sm(Fe_{0.8}Co_{0.2})_{12}$-B (70 nm)/ V (10 nm) deposited on a MgO (100) single crystal substrate. Micro-fabrication of $Sm(Fe_{0.8}Co_{0.2})_{12}$-B thin films was performed using electron beam lithography and Ar ion etching system. Finally, B, C and $B_4C$ layers were deposited. The surface morphology was characterized by scanning electron microscopy (SEM) and atomic force microscopy (AFM), the crystal structure was confirmed by X-ray diffractometer (XRD), and the magnetic properties were measured by superconducting quantum interference device magnetometer (SQUID). It was confirmed that a well-defined V/ $Sm(Fe_{0.8}Co_{0.2})_{12}$-B/ V square pattern and artificial grain boundary phase could be fabricated using the microfabrication method. The μ0Hc was increased from 1.20 T for the $Sm(Fe_{0.8}Co_{0.2})_{12}$-B continuous film to 1.39 T for the microfabricated square patterns with a B4C cap layer annealed at $T_a$ = 425 ºC. It was confirmed that the lattice constants of the 1-12 phase and subphases such as α-Fe were expanded by the addition of B and C, and this is presumed to contribute to the increase in $\mu_0 H_c$. This result demonstrates that the microstructural control is one of a possible way to understand the coercivity mechanism and also to enhance the hard magnetic properties.

## ACKNOWLEDGMENTS

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# Terahertz-Frequency Signals Generated in a Dual-Antiferromagnetic-Layer Spin Hall Oscillator

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**Abstract ID #NMM-0960**

Antiferromagnetic (AFM) materials offer unique properties that enable a variety of promising opportunities in modern science and technology, including magnetic storage, communication systems, medical imaging, neuromorphic computing, etc. Many of these applications involve the use of antiferromagnets for their ultrafast terahertz (THz) magnetic dynamics.

One of the most prominent devices for exploiting the aforementioned dynamics are spin Hall oscillators (SHOs), which consists of AFM and heavy metal (typically Pt) layers [1]. These structures provide tunability of their operating frequencies by changing the value of the DC driving current flowing through the Pt layer. However, this advantageous feature hides a significant bottleneck of AFM SHOs, i.e., their frequencies are limited by practical current constraints. In this paper, we propose to overcome the specified difficulty by proposing a novel type of SHO, the so-called dual-antiferromagnetic-layer (DAL) spin Hall oscillator, which is an analog of a dual-free-layer spin-torque nano-oscillator made of ferromagnets [2].

We consider the DAL SHO as a Pt/AFM/S/AFM/Pt multilayer structure, where magnetic sublattices in antiferromagnetic layers are canted by the Dzyaloshinskii-Moriya interaction providing the non-zero net magnetization, and two Pt/AFM SHOs are separated by a magnetoresistive spacer S. DC drive currents in the top and bottom Pt layers excite transverse spin currents in the adjacent canted antiferromagnets, leading to the appearance of THz frequency net magnetization rotation in both the top and bottom AFM layers. This rotation is then converted into a useful signal by the tunneling or giant magnetoresistance effects (depending on the spacer S material).

In this work, we numerically solve a system of the Landau-Lifshitz-Gilbert-Slonczewski equations for the net magnetizations in the AFM layers using parameters from [1] and dipolar coupling terms from [2] and investigate the behavior of the DAL SHO biased by DC drive currents applied to the top and bottom Pt layers. We performed a Fourier analysis of the net magnetization dynamics and found that the considered nanostructure can operate at either the sum (ft + fb) or difference (ft – fb) frequencies, where ft and fb are the frequencies of net magnetization rotation in the top and bottom AFM layers, respectively. Our calculations indicate that for a practically acceptable current density of 3.5·108 A/cm2, the working frequency of the DAL SHO should be about 1 THz, while the working frequency of the conventional AFM SHO from [1] does not exceed ~ 0.5 THz for the chosen current density.

We believe that the proposed DAL SHOs could be used for development and optimization of antiferromagnetic spintronic devices operating at frequencies above 1 THz, such as signal sources, detectors, modulators, etc.

## ACKNOWLEDGMENTS

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# Low-Detectable-Power Cooled Terahertz-Frequency Signal Detector Based on an Antiferromagnetic Tunnel Junction

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**Abstract ID #NMM-0963**

Pure antiferromagnetic spintronic nanostructures, consisting only of antiferromagnetic layers without ferromagnetic layers, exhibit (sub-)terahertz (THz) magnetic dynamics suitable for many promising applications in medicine, communications, security, ultrafast neuromorphic electronics, etc. [1]. One of the most developed and practically important field of the antiferromagnetic spintronics is the detection and characterization of THz signals in the signal detectors based on antiferromagnetic spintronic nanostructures of various designs [1, 2], including the detectors based on an antiferromagnetic tunnel junctions (ATJs) [3].

In this work, we extend the previously developed temperature-dependent model of an ATJ-based signal detector [4] by choosing the better matching conditions between the detector and an external electrodynamic system (transmission line, antenna, etc.) and by considering a stronger temperature dependence of the tunneling anisotropic magnetoresistance ratio [5]. Then, using this model we numerically calculated the output dc voltage Vdc , the signal-to-noise ratio SNR = Vdc / Vnoise and the minimum detectable ac power Pmin (defined as the ac signal power for SNR = 1) for the detector operating in the presence of thermal noise, and found that the minimum detectable ac power Pmin can drop to about 20 pW or less at liquid helium temperature for a detector operating at low THz frequencies ~ 0.2 THz. At the same time, the power Pmin increases at lower or higher THz frequencies. We determined that this behavior arises due to the interplay between the effect of temperature on the geometrical and electrical characteristics of an ATJ, and this effect on the impedance matching conditions. Our study indicates that depending on the junction materials and geometry, the nonmonotonic frequency dependence of Pmin can be altered, which can be used for the optimization of practical parameters of ATJ-based detectors.

We believe that the proposed formalism could be used for development and optimization of antiferromagnetic spintronic devices based on ATJs.

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# Non-resonant Spin-Torque Microwave Detector Having $L1_0$ Free Layer with Perpendicular Magnetic Anisotropy

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**Abstract ID #NMM-0970**

Spin-torque microwave detectors (STMDs) are multilayer nanoscale spintronic devices – spin diodes – that generate an output DC voltage under the action of an input AC signal. They were first experimentally implemented and studied approximately 20 years ago [1] and have a great potential for applications in various fields of modern microwave technology, such as for Internet of Things applications [2].

STMDs can operate in different regimes, one of which is the conventional resonant regime [1, 2], while the other known regimes are non-resonant, which can be suitable for energy harvesting applications [2-4]. Typically, the non-resonant regime of STMD operation is achieved for the device biased by a DC magnetic field [3] or for the device with the perpendicular magnetic anisotropy of the 1st and 2nd order of the free layer [4]. Both of these approaches to achieve a non-resonant behavior of an STMD have some drawbacks. For instance, the need for a bias magnetic field for proper STMD operation [3] prevents the creation of a "field-free" device, while the detector that has the perpendicular magnetic anisotropy of the free layer [4] requires a high-quality fabrication technology (the appearance of anisotropy is the interfacial effect).

In this work we consider an alternative design of an STMD, where the free layer is made of $L1_0$ material and characterized by a relatively weak uniaxial perpendicular magnetocrystalline anisotropy. We theoretically and numerically analyze the magnetic dynamics in an STMD without a bias DC magnetic field and estimate the output DC voltage of the detector $V_{dc}$ as a function of the amplitude and frequency of the input AC signal. Our study indicates that relatively weak uniaxial perpendicular magnetocrystalline anisotropy of the free layer leads to the reduction of detector threshold current ($V_{dc} \neq 0$, if the signal amplitude exceeds the threshold). We believe that the proposed effect could be used for the development and optimization of novel STMDs based on $L1_0$ materials.

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# Analysis of Leakage Magnetic Field of Rectangular Shaped Defects in Magnetic Materials and Investigation of Magnetic Fluids in the Field

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**Abstract ID #NMM-0974**

Magnetic Particle Inspection (MPI) is a non-destructive testing (NDT) technique that is widely used in industry to detect surface and sub-surface flaws in ferromagnetic materials. Magnetic particle inspection is a simple, fast, and cost-effective technique used in industry, particularly in evaluating the integrity of welds and critical parts. Detecting surface and sub-surface defects in ferromagnetic materials is essential for ensuring product quality, safety, performance, and regulatory compliance across various industries. Therefore there is an ongoing research on this area focused on production and use of magnetic particles, development of optical, magneto-optical, acoustic sensing methods [1,2]. Especially for magnetic particle non-destructive testing method the forces acting on particles are important. Hence the magnetic field and its gradient of rectangular prism shaped defects in a ferromagnetic material were analyzed. The magnetic fields were calculated by using analytical equations [3,4]. Magnetic field of 2x7x19 mm sized permanent magnet was measured by using a gaussmeter and theoretical results were verified. Afterwards, these analyses were used to interpret the forces acting on the non-interacting micro to nano sized particles and magnetic fluid shape on the crack indication regions. It is found that the force on a spherical magnetic particle on magnetization direction is increasing with defect width but on the perpendicular direction is decreasing. The EFH-1 light hydrocarbon-based magnetic fluid with an average particle size of about 11.6 nm was used to experimentally study a 2x2x100 mm crack on a solid magnetic material. The distribution of the magnetic fluid on the crack was studied for different heights and magnetic field values. For the layer of 2 ml EFH-1 at 2-3.5 mm height from the magnetized material, around 3.7-5.0 mm width of nearly Gaussian shape of fluid is observed. The experimental results are discussed with theoretical analysis.

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# Magnetic Properties of Sol-gel produced Cerium substituted YIG thin film

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**Abstract ID #NMM-1003**

Yttrium-iron garnet (YIG) and its substituted derivatives are highly preferred in many applications of magnetics due to their outstanding properties in RF circuits and magneto-optics [1]. Cerium-substituted YIG (Ce:YIG) is a material with superior magneto-optical properties, making it a focus of ongoing research efforts [2].

This study investigates Ce:YIG thin films deposited on Si(100) substrates using the sol-gel technique with a yttrium/cerium molar ratio of 2.8/0.2. The as-deposited films were heat-treated at 800°C to obtain Ce:YIG films exhibiting optimal properties. The film thickness was measured to be 300 nm. A photoelastic modulator-based Kerr magneto-optical measurement setup was designed and used to characterize the films. The results of the magneto-optical setup were compared to the magnetic properties obtained from a vibrating sample magnetometer (VSM). FMR measurements were taken at angles between 30° and 90°. The analysis of the resonance angle dependence through FMR revealed the linewidth parameter ranging from 21.89 to 40.66 mT. The FMR results were discussed by comparing them to previously published ones. The results of the linewidth parameters are found to be larger than many YIG materials produced by other methods [3–4]. The broader linewidth observed was attributed to crystallinity and impurities in the produced Ce:YIG thin film.

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# Focused Ion Beam Parameters Influence on Magnetic Properties of the Nanostructures

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**Abstract ID #NMM-1012**

This work investigates the impact of Focused Ion Beam (FIB) technology on the magnetic properties of materials [1] for the fabrication of optimized magnetic structures in magnonics applications. Utilizing a combination of experimental techniques and numerical simulations [2], the research aims to enhance the precision in the fabrication of magnetic nanostructures specifically tailored for magnonic functions, thereby advancing the field of magnetic nanostructure technology.

Central to this study is the exploration of FIB's capabilities in magnetically isolating sections of materials without physical separation [3]. This focus includes an assessment of the precision of magnetic modifications using FIB, which is supplemented by ion influence estimations via SRIM software and further supported by empirical FIB experiments. These experiments explored various factors, including the influence of the FIB's built-in tools, beam direction, and mask optimization strategies to prevent overexposure.

The work then addresses the practical implementations of these findings in magnonics, drawing upon the insights gained and additional experimental work. This holistic approach is expected to significantly contribute to the domain of magnetic nanostructures, offering new insights and methodologies that could propel further research and applications in magnonics and related fields.

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# Flexible Hair Tactile Array Based on Micro Magnetic Particles

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**Abstract ID #NMM-1022**

Tactile sensing is an essential modality for humans to perceive the external environment. With the increasing popularity of household robots, precise grasping and safe human-machine interaction have become increasingly important. A crucial way to solve these problems is to endow robots with large-area tactile perception capabilities. In recent years, tactile sensors based on various principles have been developed. Among them, tactile sensors based on magnetic principles have the advantages of high resolution, low mechanical hysteresis, and non-contact measurement. In addition to film and convex structures, tactile sensors with hair structures have also been developed, which can greatly increase device sensitivity [1-2]. However, these studies often use a single hair or a small amount of hairs to achieve single-point measurement [3]. Therefore, it is difficult to apply them in robot skin or other fields requiring large-area perception, and it is also difficult to achieve complex functions.

In this paper, we propose a magnetic hair array with tactile sensing ability. Every hair in the array contains a large number of micro magnetic particles. When the external force acts on the hair array, multiple hairs will bend under the force. At this time, the size and direction of the stray magnetic field under the hair array will change. The magnitude and direction of the external force can be calculated by detecting this change through the magnetic sensor array under the hair array. The magnetic hair array is then applied to sliding tactile sensing and object recognition. It can realize precise detection of the size, direction, and sliding of external force and achieves a success rate of 97% in object recognition. In addition to recognizing the shape of objects, the magnetic hair array can identify whether the object has magnetism inside, which has great application potential in intelligent robots and rescue relief in the future.

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# Quaternary Dilute Ferromagnetic Semiconductors for Photonic and Spintronic Applications

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**Abstract ID #NMM-1033**

Dilute ferromagnetic semiconductors (DFMSs) are a class of alloys that merge semiconductor traits with magnetism within a single material. These amalgamations of electronic and magnetic characteristics give rise to entirely fresh physical attributes, which are intriguing for fundamental research and exhibit potential for a broad spectrum of spintronic devices lies in their ability to generate spin-polarized currents. Besides the generation of spin current, which is pertinent to spintronics, it is anticipated that modifications in the band structure due to the presence of additional doping ions such as In, P, or Bi in the (Ga,Mn)As matrix will engender innovative DFMS device concepts [1-3]. Integrating the heavy Bi or In atoms, substituting As atoms in epitaxial GaAs layers, leads to a pronounced enhancement of the spin-orbit interaction in the valence band. The spin-orbit coupling engenders numerous phenomena in magnetic materials such as (Ga,Mn)As, including anisotropic magnetoresistance (AMR), planar Hall effect (PHE), and spin-orbit torque. The (Ga,Mn)(P,As) epitaxial layers on GaAs thus harbor ferromagnetism with perpendicular magnetic anisotropy, rendering them suitable for observing crucial phenomena such as the anomalous Hall effect (AHE).

We have investigated 30-nm-thick $Ga_{1-x}Mn_xPyAs_{1-y}$ layers doped with x = 0.08 of Mn and y = 0.12 - 0.32 of P, 100-nm-thick $Ga_{1-x}Mn_xBi_yAs_{1-y}$ with x = 0.04 of Mn and y = 0.003 of Bi, and 30-nm-thick $InyGa_{1-y-x}Mn_xAs$ with y = 0.03 of In and a Mn content x ranging from 0 to 5.6%, grown on (001)-oriented GaAs substrates at 230°C by low-temperature molecular-beam epitaxy.

X-ray diffraction (XRD) and transmission electron microscopy (TEM) confirmed the crystalline quality of the layers' sharp interfaces with the substrate. The magnetic properties and the Curie temperature (TC) of all Mn-doped layers were determined by superconducting quantum interference device (SQUID) magnetometry. μ-Raman spectroscopy was used to estimate the hole densities in the Mn-doped layers. The optical properties of the layers were measured by spectroscopic ellipsometry (SE) and modulation photo-reflectance spectroscopy (PRS) [4, 5].

The post-growth low-temperature annealing of the layers has been shown to enhance their Curie temperature, accompanied by an increase in the free hole concentration. The spectroscopy results are consistent with the valence-band model of hole-mediated ferromagnetism in the (Ga,Mn)(Bi,As) and (In,Ga,Mn)As layers. They reveal a downward shift of the chemical potential for Mn-doped GaAs, Ga(Bi,As) and (In,Ga)As, and a highly dispersed band crossing the Fermi level. It is found that Bi and In ions cause significant modifications to the spin-split-off band. The optical gap of as-grown (Ga,Mn)(As,P) is slightly smaller than that of Ga(As,P). These observations can be interpreted by considering an Mn impurity band that pins the Fermi level above the valence band edge in as-grown samples.

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# Exploring the Optical and Magnetic Properties of Molecular Beam Epitaxy-Grown Diluted Multicomponent III-V Semiconductor Nanofilms

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**Abstract ID #NMM-1038**

Dilute multicomponent semiconductors represent a class of alloys that integrate semiconducting properties with ferromagnetism or superconductivity. This combination of electronic and ferromagnetic or superconducting properties yields novel physical characteristics that are intriguing for both fundamental research and practical device applications. Tailoring the band structure through the introduction of additional doping ions such as P, In, or Bi in the III-V semiconductor matrix [1–3] enables the exploration of innovative device concepts.

For this study, we present a comprehensive investigation into the relevant physical properties of dilute multicomponent III-V semiconductor nanofilms. This investigation employs a combination of analytical techniques including Fourier-transform infrared spectroscopy, spectroscopic ellipsometry (SE), high-resolution X-ray diffraction (HRXRD), micro-Raman spectroscopy, SQUID magnetometry, and broadband ferromagnetic resonance spectroscopy (VNA-FMR).

This multifaceted approach allows for the determination of key magnetic and optical characteristics of the material, such as dielectric functions, band structure, Curie temperature, saturation magnetization ($M_s$), anisotropy fields (crystallographic cubic $H_c$ and uniaxial $H_u$), axes and planes of easy magnetization, ferromagnetic resonance line width (ΔH), Gilbert damping constant (α), and more. A thorough understanding of the magnetic characteristics of the samples facilitates the realization of the full potential of ultra-thin III-Mn-V semiconductors and topological semimetals for applications in magnetic storage and microwave technologies [4,5].

Specifically, our focus lies on quaternary (Ga,Mn)(P,As) compounds with varying P (up to 32%) and Mn (up to 8%) content, as well as SnInTe with different In (up to 30%) content epitaxial layers grown by molecular beam epitaxy (MBE) on p-type and semi-insulating (001) GaAs substrates. The absorption infrared spectrum was measured using a Nicolet 380 spectrometer (Thermo Fisher Scientific), collecting high-resolution spectral data over a wide range from 400 to 4000 $cm^{-1}$. These measurements were complemented by SE-2000 Semilab multi-angle spectroscopic ellipsometer readings (working wavelength range: 250 nm to 2100 nm).

Additionally, the crystalline quality of the layers and sharp interfaces with the substrate were confirmed using HRXRD, revealing the pseudomorphic growth of very thin nanofilms on (001) GaAs. Composition analysis of the thin films was conducted using secondary-ion mass spectrometry (SIMS) and Auger electron spectroscopy (AES).

Micro-Raman spectroscopy was employed to estimate the free hole densities in the nanolayers. By combining the aforementioned experimental methods, we could precisely define the band structures of the epitaxial layers and identify additional impurity states within the band gaps.

**ACKNOWLEDGMENTS**

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# Fundamental Preparation of Polylactic Acid Self-assembled Monolayers for Future Spintronic Applications

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**Abstract ID #NMM-1044**

The cumulative effect of atoms in chiral molecules can lead to spin polarisation, so that an electron passing through a chiral molecule is spin polarised. Such molecules act as spin filters [1]. Control of the electron spin is crucial in spintronics, and the use of such spin filters in spintronics has been shown to have advantages such as lower energy consumption, scalability or the introduction of phase changes [2, 3]. However, the generally accepted theory behind the effects induced by chiral molecules has not yet been developed. There is a strong need for experiments on effects associated with chiral induced spin selectivity, using different materials as well as different polymers.

Our work has focused on the preparation of self-assembled monolayers based on chiral polylactide acid on prepared heterostructures. Heterostructures consisted of ferromagnetic perovskite La1-xSrxMnO3 with few nm of Au on the top, deposited on a monocrystaline SrTiO3 substrate. Polylactid acid creates an alpha-helix in which chiral induced spin selectivity is expected to occur. Such polymers are inexpensive and easy to modify with a simple chemical formula. This makes them suitable for both industrial and research applications. We used the thiol functional group of modified chiral polylactic acid to create self-assembled monolayers on gold. We expect our work to be a stepping stone for future research and possible applications in organic-based spintronics, as we show that such chiral monolayers influence the properties of the underlying material.

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# Canted Antiferromagnetism in Two-dimensional Altermagnets

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**Abstract ID #NMM-1050**

Receiving increasing interest in the field of spintronics are a type of magnets known as altermagnets [1,2], which exhibit zero net magnetization and feature spin-split electronic bands. Using the combination of the density functional theory and symmetry analysis we show that RuF4 monolayer is a two-dimensional d-wave altermagnet [3]. Furthermore, we show that spin-orbit coupling has a pronounced effect on the splitting of the electronic bands of RuF4, giving rise to pronounced spin splitting of the electronic bands at the Γ point by ∼100 meV and turning this material into a canted antiferromagnet. We explain the appearance of canted antiferromagnetism and the spin splitting at the Γ point using the group theory and extend our analysis to other two-dimensional altermagnets (VF4, AgF4, OsF4, FeBr3) recently discovered [4]. Finally, we argue that the canted antiferromagnetism in two-dimensional altermagnets gives rise to the Rashba-Edelstein effect which could be easily detected in charge-spin conversion experiments [5].

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# Towards Magnetically Ordered Artificial Spin Crystals

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**Abstract ID #NMM-1102**

Motivated by the possibility of the existence of topologically protected and unidirectional magnetic waves [1,2], we address the topic of artificial magnetic crystals. Translational symmetry is a basic prerequisite for the existence of a band structure of waves. Current nanotechnology enables the fabrication of nanostructures with the properties of crystals. The problem of a magnetic artificial crystal is, in addition to the production of a periodic magnetic pattern, also the achievement of periodically repeating magnetization. For our purpose, we need a circulating arrangement of magnetization in a periodically repeating unit cell. Individual elements of our magnetic crystal interact only through dipole-dipole interaction. Unlike artificial spin ices, our structure is not frustrated and has a known ordered ground state. Nevertheless, it is difficult to achieve a ground state due to the high energy barrier when changing the polarity of individual elements. This is a well-known problem and reason for the impossibility of performing temperature annealing of magnetic systems. In this work, we present several strategies for achieving the ordered state of a magnetic crystal with circular arrangement in the unit cell as well as the numerical method for calculation energy barriers and minimum energy paths [3].

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# Enhancement of Damping in YIG films at MilliKelvin Temperatures due to GGG Substrate

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**Abstract ID #NMM-1111**

Magnonics is the field of science that deals with data carried by spin waves and their quanta, magnons, in magnetically ordered media [1]. The ferrimagnet yttrium iron garnet (YIG) $Y_3Fe_5O_{12}$ is the material with the lowest known magnetic damping [2] and therefore often used in experiments and RF technologies. The use of YIG films of thicknesses down to tens of nanometers grown on gadolinium gallium garnet (GGG) $Gd_3Ga_5O_{12}$ substrates [2] enables the development of magnetic devices and circuits at the nanoscale [3]. Recently, the field of quantum magnonics, operating with single magnons and versatile hybrid structures at millikelvin temperatures, attracts significant attention [3]. However, it is known that lowering the temperature increases the magnetic damping of YIG, which is usually associated with the influence of the paramagnetic GGG substrate [4].

In this work, we measured a 97 nm-thick YIG film grown on 500 µm-thick GGG substrate and cut into a quadratic chip with an edge length of 5 mm. We have performed stripline ferromagnetic resonance (FMR) spectroscopy up to 40 GHz, using a physical property measurement system (PPMS), operating at the temperatures between 2 K and 300 K and a dilution refrigerator capable of reaching temperatures of 10 mK. The measurements were performed in in-plane orientation of the external magnetic field. To determine the magnetization of GGG in the temperature range from 2 K to 300 K, we have performed vibrating-sample magnetometry (VSM) on a pure GGG slab ($M^s_{GGG}$ = 805 kA/m). At low temperatures, the GGG can be saturated to a significantly high value of hundreds of kA/m when magnetic fields of several hundred mT are applied. Our FMR studies show that at temperatures below 50 K and externaly applied fields the paramagnetic GGG is sufficiently magnetized and induces a stray field in the YIG layer.

The induced field is highly inhomogeneous and opposes the externally applied field for the in-plane geometry. The lower the temperature and the higher the external fields, and therefore the higher is the stray field induced by the GGG, which naturally creates a shift in frequency of the FMR [5]. The FMR linewidth ΔB, which is a measure of magnetic damping in the system increases for lower temperatures and is more than eightfold at 2 K compared to room temperature. The stray field induced by the GGG is very inhomogeneous over the area of the YIG film [5], and is therefore one contribution of the anomalous increase in linewidth at low temperatures, confirmed by comparing the experimental results with specialized micromagnetic simulations. However, the magnetic system of the YIG can couple with other dissipation channels that occur at low temperatures. For instance: (1) YIG/GGG exchange and (2) dipolar coupling, (3) heavy-metal impurities. A better understanding of these ultralow temperature damping mechanisms will pave the way for quantum magnonics on thin YIG films.

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# Functional Nanostructured Cu-based Alloys with Shape Memory Effect and Tunable Magnetic Properties

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**Abstract ID #NMM-1114**

Functional materials play an important role in many applications to solve a variety of specialized problems by actively providing functionality through their properties. Shape memory alloys are excellent candidates for solid-state actuation and thermal energy harvesting applications due to their capability to undergo reversible solid-to-solid martensitic phase transformations, with tailorable shape change and energy conversion capabilities. Magnetic shape memory alloys (MSMAs) are of great interest for creating fundamentally new designs of actuators, sensors, functional microdrives, power devices, and technologies [1-4].

The development of nanostructured Cu-Al-Mn alloys with tunable magnetic-mechanical properties is an important challenge in the emerging field of functional materials enabling fast large-strain actuators. Introducing magnetic anisotropy into nanoparticles can be an effective method to obtain new properties and functions crucial for many applications. Depending on the size and distribution of nanoparticles, Cu-Al-Mn alloys can exhibit spin glass, superparamagnetic, ferromagnetic, and antiferromagnetic ordering. Cu-Al-Mn alloys show large elastic anisotropy, which stimulates the increase in magnetic anisotropy. Our experiments showed that the elastic stresses under martensite transformation (MT) induce large magnetic anisotropy, with one to two orders of magnitude larger than the magneto-crystalline one.

This study is devoted to a comparative analysis of structural and magnetic characteristics of Cu-Al-Mn alloys under thermomagnetic treatment (TMT) such as aging in a magnetic field of 1.5κOe at $T$=200°C resulting in ferromagnetic nanoparticle precipitation. Using a complex of magnetic and structure investigations, the structural phase transition of martensitic type and magnetic transitions: paramagnetic-superparamagnetic-spin glass were studied in a wide temperature range. A decrease in magnetic moment and an increase in coercivity has been noted accompanied by a slight shift in temperatures of magnetic transitions in case of aging in parallel magnetic field in comparison with a sample without field. Changes in magnetic quantities are explained by additional induced magnetic anisotropy resulting from TMT and MT.

## ACKNOWLEDGMENTS

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# Ferromagnetic-like Behavior of Ethanol Solutions of the ZnO Nanoparticles

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**Abstract ID #NMM-1126**

The ethanol solutions of the ZnO nanoparticles were placed in a constant and homogeneous weak magnetic field ($B$ = 60 mT). Exposure time in the field was: 1 hour, 1 day and 5 days. These solutions were used for photocatalytic formation of ZnO/Ag nanoheterostructures under the action of UV irradiation. The production cycle was repeated during 30 days. During this time, the evolution of the obtained optical absorption spectra of solutions containing ZnO/Ag nanoparticles were measuredrelative to a cuvette with pure ethanol. For reliability of the received results the solution which was not exposed in magnetic field, but stored together with all samples at the same temperature conditions was used as a reference. Under the UV action, photocatalytic reduction of Ag (I) and the formation of a ZnO/Ag colloidal heterostructure occurs, which is characterized by an absorption maximum at 400–460 nm. Moreover, increasing the UV dose leads to a long-wavelength displacement of this peak. These processes are characteristic for all studied samples. But the energy positions of the observed peak at low and maximum doses of weak magnetic field radiation do not match. It was found that within 30 days the final position of the maximum of plasmon absorption of the Ag nanoparticles, which were formed on ZnO solutions, that have been undergone magnetic field treatment, slowly shifts to the position of the latter in the reference sample. The latter circumstance indicates a "memory effect" that lasts for a month.

The ferromagnetic-like behaviour of ZnO NPs ethanol solutions appears itself in the fact that the magnetization was held after the exposition in the magnetic field. Such features can be caused by the spins of unpaired electrons located on the surface of nanoparticles. It is well known that the surface for nanoparticles plays a significant role. Two circumstances that have been detected are unusual: firstly, it is a very long duration of magnetization, which lasted on the order of a month, and secondly, it is generally the fact of the existence of ferromagnetic properties in non-magnetic substances. Direct measurements of magnetic properties of non-doped ZnO NPs were done in [1, 2]. These results confirm our assumptions.

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# Creation of the Magnetic Skyrmions by the Stray Fields Produced by Superconductor Ring

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**Abstract ID #NMM-1157**

Magnetic skyrmions are topologically non-trivial magnetization configurations. In recent decades, skyrmions have attracted much attention due to their potential applications such as racetrack memory, microwave oscillators and logic nanodevices. Conventionally, magnetic skyrmions are stabilized by the Dzyaloshinskii-Moriya interaction (DMI), which imposes rather strong constraints on the choice of magnetic materials. Here, we propose an alternative approach to generate the skyrmion by the inhomogeneous field produced by superconducting (SC) nanostructure placed in the vicinity of the magnetic system, made of the material which does not exhibit DMI.

In the Meissner state, the eddy currents in a SC nanostructure shield its interior from the external magnetic field by forming a stray magnetic field outside the SC system. The stray field can be controlled by both the external magnetic field and the time-dependent electric field. When the magnetic system is located in the vicinity of the SC nanostructure, the stray field of the superconductor can influence the magnetization dynamics. In our work, we theoretically investigate the creation of magnetic skyrmions in a uniform magnetic layer by the stray field of an SC ring.

The hybrid system under study consists of a Ga:YIG ferrimagnetic (FM) thin film and a flat SC ring made of Nb. In Ga:YIG, the shape anisotropy is overcome by the out-of-plane anisotropy, leading to the out-of-plane orientation of the magnetization. We have considered two cases: a) the system is placed in an external magnetic field perpendicular to the FM layer and eddy currents are induced in the SC ring b) the electric field pulse is applied to the SC ring to create a unidirectional superconducting current. In both scenarios, the eddy currents in the SC create a non-uniform distribution of the magnetic field with radial symmetry in the FM film, which is favorable for the appearance of Neel-type skyrmions.

We did not consider the impact of the FM layer on the SC strip. Our studies were carried out in two steps. First, we calculated the static stray field generated by the SC strip. It was determined from the distribution of SC currents, which was found by semi-analytical solution of the London equation [1]. The stability and sizes of the skyrmion in the magnetic film are calculated taking into account the SC stray fields (Zeeman interaction), the exchange interaction, the magnetostatic interaction and the out-of-plane magnetic anisotropy. The generalized DeBonte ansatz [2] is used to describe the inhomogeneous skyrmion magnetization.

## ACKNOWLEDGMENTS

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# Geometry-Governed Effects in Curvilinear Magnetism: Fundamentals and Applications

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**Abstract ID #NMM-1162**

The onrush of nanotechnologies extended conventional flat architectures to curved space, showcasing the fundamental importance of the mutual interplay between geometry, topology and the order parameter. In the case of magnetism a mutual interplay of magnetization texture (material properties), curvature, and topology (geometrical properties) becomes a playground for curvilinear magnetism [1]. By tailoring curvature and topology of the conventional magnetic materials there appears a possibility to control material response leading to modification or even launching new functionalities [2]. This is granted by complementary expertise and advances of fundamental researched, materials sciences and technologies.

This talk focuses on the peculiarities emerging from geometrically curved magnetic objects, including 3D bent and twisted curved wires and films. The curvilinear geometry manifests itself in emergent interactions. These geometry-governed interections can be local driven by exchange and stemming from local curvature and torsion [3] or stemming from the varying cross-section [4], but also can be nonlocal driven by magnetostatics and supported by topology [5]. As a consequence, family of novel geonetry-governed effects emerge, which include magnetochiral effects and topological patterning, resulting in theoretically predicted domain wall automotion, unlimited domain wall velocities, chirality symmetry breaking, mesoscale Dzyaloshinskii-Moriya interaction etc. Current and future challenges of the curvilinear magnetism will be discussed.

## ACKNOWLEDGMENTS

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# The Anomalous Inverse Spin Hall Effect and the Field-free Switching of YIG

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**Abstract ID #NMM-1167**

Conversional spin-charge interconversion such as the (inverse) spin Hall effect and (inverse) Rashba-Edelstein effect requires the propagation direction, spin polarization direction of the pure spin current and the electric current direction to be orthogonal to each other. Recent theory predicted that this constrain can be removed in the effects termed as the anomalous (inverse) spin Hall effect (ASHE and AISHE) in ferromagnetic metals [1].

We present the experimental demonstration of these effects. With the spin pumping measurements, we find the converted charge current in perpendicular magnetized Co/Pd multilayers can be either perpendicular or collinear with the spin polarization, depending on the injecting spin current spin polarization direction. With the latter case, the sign and magnitude of converted charge current can be linearly regulated by the out-of-plane magnetization [2]. With the spin Seeback effect measurements, we show that both the perpendicular and collinear spin current generated by a perpendicular magnetized Yttrium iron garnet (YIG) can be converted into charge currents in the in-plane magnetized Permalloy (Py). And vice versa, with a charge current applied in the in-plane magnetized Py, both the orthogonal and collinear spin currents can be generated and further used to perform the field-free switching of the perpendicular magnetized YIG [3]. These studies reveal the interesting features of the spin-charge interconversion in ferromagnetic metal, in excellent agreements with the theory [1]. They also open an avenue for the highly efficient field free switching without heavy metal.

## ACKNOWLEDGMENTS

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# Magnonic Inverse-Design Processor

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**Abstract ID #NMM-1174**

The field of magnonics, in which magnons, the quanta of spin waves, carry and process information, has shown promise for energy-efficient data processing [1]. Recently, several proof-of-concept magnonic devices have been developed using inverse design [2-4]. In inverse design, a functionality is first defined and a feedback loop algorithm provides a configuration in a complex reconfigurable magnonic medium to achieve this functionality [2]. The drawback of the previously reported approaches is that the inverse problem has to be solved numerically first, which can be time and energy consuming depending on the complexity of the functionality, and only afterwards the obtained design can be reproduced experimentally [4]. In addition, a perfect calibration between numerics and experiment is required. Here we report on a conceptually different approach where the inverse problem is solved experimentally [5].

The experimental magnonic universal unit is based on an 18-um-thick YIG rectangular film with 7x7 omega-shaped DC loop array placed on the YIG film. The loops are connected to 49 independent current source channels with currents limited to the range of -300 to +300 mA. Three input and three output antennas are used to access a wide range of functionalities. A biasing magnetic field is applied normal to the YIG surface.

A genetic optimization algorithm is used to implement the notch filter functionality. After a random initial population, the algorithm creates a new generation (set of current values) by crossing over the best-performing parents (selection rules) and introducing mutations to individual parents to form children. Experimentally, the algorithm sets the value for each current source channel and then commands the VNA to measure the spectra corresponding to the current configurations. The transmission data is sent back to the PC, and the optimizer calculates the objective value that maximizes the losses in the filter range while minimizing any changes outside the filter range.

Through our work, we have demonstrated the processor's capabilities by realizing RF filter and demultiplexer functionalities [5]. Our filter function achieved significant attenuation in the rejection band, reaching approximately 10^5. Similarly, the demultiplexer function exhibits a high attenuation of approximately -40dB within the defined frequency ranges for the corresponding outputs. The proposed magnonic media can potentially be reconfigured on the time scale of a nanosecond. With its intricately designed reconfigurable region, we are confident that our processor can achieve various other functionalities for RF applications for 5G and 6G, logic gates, or neuromorphic computing.

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# Nanoscale Ga:YIG-Based Magnonic Crystals

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**Abstract ID #NMM-1175**

Spin waves (SW) offer significant potential for both fundamental and applied research owing to the scalability, tunability and energy efficiency inherent in magnonic devices. These prototypes are often realised based on one-dimensional (1D) micrometre-large magnonic crystal (MC) – artificial magnetic materials with a spatially periodic variation of properties. However, in order to surpass modern technology, MCs should perform reliably already in the sub-micrometre range [1]. To achieve this one can operate with nanostructures in a single-mode regime [2], where the prominent exchange interaction causes the unpinning of SW modes and their further quantization on the frequency axis – a promising, yet challenging fabrication task.

Recently, due to the progress in material physics and fabrication approach, we have realised 1D MCs for efficient control of single-mode SW transport. Nanostructures were developed from the 100 nm-thick epitaxial films of a reference $Y_3Fe_5O_{12}$ (YIG) and $Y_3Fe_{5-x}GaxO_{12}$ (Ga:YIG, Gax $\approx$ 0.9) based on our previous studies [3], that revealed a small Gilbert damping ( $\alpha \approx 6.1 \cdot 10\text{-}4$), isotropic dispersion relation and fast exchange SWs in out-of-plane Ga:YIG films. Magnonic crystals were fabricated by means of electron beam lithography, ion etching and evaporation. Width-modulated and antidot-based 1D MCs have a periodicity of 1 μm with the number of periods $N_a$ (200) between the input and the output antennas; notches' depth x and diameter of the antidots dx were used for the optimization. The SW dispersion allowed for the estimation of the (relative) positions of the band gaps in the magnonic spectrum. Based on the simulations, the best performance (best ratio of minimised losses to well-defined band gaps) is expected for the 1D MC with notches of depth $x$ = 100…200 nm and with holes of diameter $d_x$ = 150 nm.

Micro-focused Brillouin light scattering spectroscopy and propagating spin-wave spectroscopy were used to experimentally investigate SW transport. In addition, magnetisation dynamics were studied using micromagnetic simulations with mumax3 software.

Obtained results pave the way for the MC designs of more advanced functionality – 2D arrays with magnon guiding via defects, reconfigurable and dynamic MCs. Moreover, they are important in the light of the possibility to realise topologically-protected magnonic transport in 2D MCs – a scientific challenge, that has never been realised experimentally yet [4].

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Current results on the nanoscale magnonic crystals are of high novelty and are part of the on-going research within FWF ESPRIT Fellowship Grant ESP 526-N TopMag „Nanoscale Topological Magnonic Crystals".

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# Multi-Input Programmable Artificial "Neuron" Based on Antiferromagnetic Spintronic Nanostructures

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**Abstract ID #NMM-1178**

Artificial neurons and neural networks based on them are now considered to be the key elements required for the implementation of artificial intelligence. There are many types of artificial neurons and neuron-like systems capable of mimicking the behavior of biological neurons in a brain, including the recently proposed "neurons" based on antiferromagnetic (AFM) spin Hall oscillators (SHOs) [1]. Such AFM-based "neurons" are capable of generating "Dirac-delta-like" pulses (spikes) of ~ 1 ps duration under the action of input AC and DC signals, but their real-time programming has not yet been considered, which greatly slows down the development of practical AFM-based neural networks. In this paper we consider an approach to implement an AFM-based programmable "neuron" ("P-neuron") as a simple two-layer neural network consisting of several single-input AFM-based conventional "neurons".

We consider each of the AFM-based "neurons" as a Pt/NiO/Pt SHO driven by the DC and AC currents applied to the single Pt contact of the spintronic structure [1, 2]. The input DC current defines the working state of the "neuron", while the input AC current of sufficient amplitude can initiate the rotation and reversal of the magnetic sublattices of the AFM NiO layer of the spintronic structure used [1, 2]. This motion of the AFM magnetic sublattices, in turn, leads to the generation of an output current spike that propagates in the second Pt layer.

Although the considered Pt/NiO/Pt spintronic structure can have multiple inputs, its bottleneck is the method of specifying the working point of the system by choosing a particular value of the input DC current applied to the "neuron". The state of the "neuron" is actually defined by the total DC current applied to all inputs, which makes it difficult to reconfigure the "neuron" in real time by changing the DC currents applied to different inputs (if their sum is the same). In contrast, in this paper we consider another approach that may be suitable for implementing an AFM-based "P-neuron". Such a "P-neuron" is a two-layer neural network, where each conventional AFM-based "neuron" in the first input layer has only one but independent input. The state of each of the first-layer "neurons" can be changed independently by applying a particular bias DC current that affects the "neuron's" working point. All outputs of the first-level "neurons" are connected to a single multi-input "neuron" forming the second layer of the considered "P-neuron". We found that by applying different DC currents to different inputs of the "P-neuron" one can change the "sensitivity" of the "P-neuron" to AC signals coming from these signal inputs, i.e. one can implement a programmable AFM-based artificial "neuron".

We believe that the proposed programmable AFM-based artificial "neurons" and their programming algorithm could be used for the development and optimization of ultrafast neural networks based on antiferromagnetic spintronic oscillators.

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# Advancing Waste-Derived Composite Material for Stealth Applications

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**Abstract ID #NMM-1193**

Advancement in telecommunication appliances raises the problem of electromagnetic interference (EMI) and electromagnetic compatibility (EMC). To address these issues, microwave absorbing materials have emerged as crucial solutions with significant implications for electromagnetic compatibility and stealth technology.

The present work focuses on synthesizing magnetic and dielectric material-based composites through a top-down approach tailored for stealth applications. The magnetic material is synthesized via the cost-effective sol-gel auto-combustion route, while the dielectric material is derived from waste. Structural and morphological analyses of the developed material have been done using X-ray diffraction (XRD), scanning electron microscopy (SEM), and Raman spectroscopy, revealing nano-sized particle distribution. Further, to explore the developed composite for electromagnetic performances, its permittivity and permeability characteristics are measured using a vector network analyzer. The absorption in the frequency, range of 8.2-12.4 GHz depends notably on the permeability and permittivity of the material. The developed material is cast into the form of rectangular pallets with the aid of binders for measuring the electromagnetic parameters. The microwave absorbing material in the 8.2-12.4 GHz frequency range plays a vital role in stealth technology. These materials are valuable in military applications such as reducing RCS, camouflaging the target, and preventing the EMI and EMC. These materials are very useful in military applications such as for RCS reduction, camouflaging of the target, and preventing the EMI and EMC.

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# Concentration and Heat Treatment Effects on Magnetoresistive Properties and Structural-Phase State of Granular $Co_xAg_{100-x}$ Alloy Thin Films

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**Abstract ID #NMM-1204**

The development and research of new magnetic films is one of the most important problems of modern nanotechnology and nanoelectronics. Magnetic nanogranular heterostructures possessing magnetoresistive effects, such as giant (GMR) and anisotropic magnetoresistance have found a wide range of applications in nanoelectronics [1] (e.g. non-volatile magnetic memory, sensors of magnitude and direction of the magnetic field, magnetic resonance tomography). The magnetotransport properties of granular alloy thin films are determined by their composition and structural state. The magnetoresistive properties of magnetic nanogranular heterostructures depends critically on various dimensional constraints such as the size and shape of magnetic granules and the inter-granulear distance. The changes in the structural parameters of the pristine material caused by the annealing process should influence the magnetotransport properties of the investigated granular thin films.

Comprehensive investigation of the nanostructure, phase state and the magnetoresistive properties of $Co_xAg_{100-x}$ alloy thin films with thickness of 20 nm in a wide range of component concentration (17 at. % $\leqslant x \leqslant$ 89 at. %) in unannealed state and after the heat treatment within the temperature range of 370 – 800 K was presented. The samples were obtained by the method of electron beam co-evaporation at room temperature. The correlation between the structural-phase state and magnetoresistive properties was established by transmission electron microscopy method. The study of unannealed samples showed the following. Different types of magnetoresistive effect were observed. At low concentration of Co (at $x < 64$ at.%) the films had a phase composition of Ag (fcc) + Co (hcp) and were characterized by an isotropic GMR. The threshold of structural percolation in granular films was observed for $x \approx 60$ at.%. Films in the unannealed state were characterized by the largest values of the magnitude of GMR. The maximum GMR values of 7.2% and 7.5% in transverse and longitudinal geometry, respectively, were observed at $x = 55$ at. %. For higher Co concentrations ($x > 70$ at. %) the films demonstrated anisotropic magnetoresistance, which is assumed to be associated with the appearance of ferromagnetic interactions between the Co granules. The process of heat treatment of film samples in the temperature range of 370 – 800 K did not cause a significant change in their phase state. The heat treatment of samples of alloy thin films caused a decrease the magnitude of GMR and an increase of the coercive force. After the heat treatment of the samples at temperature $T$ = 370 K, the magnitude of GMR decreased 1.3 times, and at $T$ = 800 K - 15 times compared to the magnitude of GMR in the unannealed state. This behaviour of the magnetoresistive properties of granular alloy thin films is determined by changes in the structural state, namely, an increase in the size of Co granules during heat treatment of the samples.

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# An Organomagnetic Smart Film

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**Abstract ID #NMM-1219**

Recent advancements in material science have placed significant emphasis on the development of materials with smart properties and functionalities that can be controlled or adjusted by external stimuli. In this study, we present a novel smart, flexible, conductive composite organic material comprising a thin layer of polydimethylsiloxane (PDMS) and polypyrrole (PPy) precursors. These materials were strategically doped with nickel nanoparticles (NiNPs) to create an Organic Magnetoresistance (OMAR) composite film[1-2].

The MR sensitivity of flexible organic composites at room temperature typically falls below 1 for millitesla-scale magnetic fields [3-5]. Our experiments demonstrate that the fabricated film exhibits notable magnetoresistance effects, with relative electrical resistance changes ($\Delta R/R0$) of 5.2 under a weak magnetic field of $10^{-2}$ T in ambient conditions. The conductivity of the composite is attributed to the presence of delocalized π-electrons, while its heightened OMAR capabilities, stable up to 5 kHz switching rates, further underscore its potential.

To investigate the magnetic permeability of the samples, we employed a custom-built time-domain magnetic spectrometer, which revealed enhanced diamagnetic behavior. This enhancement is indicative of the composite's magnetic resistance, resulting from spin injection and subsequent interaction with the magnetic field.

These promising organomagnetic self-standing layers hold significant potential for various applications, including magnetic switches, sensors, e-skin, transistors, and organic spintronic devices.

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# Domain Wall Automotion in Curved Ferromagnetic Nanostripes by Cross-section Tailoring

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**Abstract ID #NMM-1224**

Manipulation of magnetization topological textures, in particular, domain walls, is a key task of spintronics. The curvilinear magnetism [1] provides a new geometrical route of such manipulations. One of the nanoscale magnetic architectures that has become of a key interest is the curved ferromagnetic nanostripes. Although, the magnetic response of the curved nanostripe is already well-studied, in all previous studies cross section of the nanowire was assumed to be constant. Only recently, a new micromagnetic framework emerged that allows the exploration of the changes in the magnetization dynamics caused by the cross-section area gradient [2].

Here, we study theoretically how the motion of the domain walls in a curved narrow ferromagnetic nanostripe can be tailored by the spatial variation of the nanostripe cross section. The effective equations of the domain wall motion are derived and analysed in detail using the collective variable approach. The resulting equations are applicable for a wide class of nanostripe geometries and our approach is showcased by two specific examples of straight stripe and circular arc. The study of the domain wall motion shows the creation of an internal driving force by the gradient of the cross-section area of the curved ferromagnetic nanostripe and can explain the recent experimental results [3]. This force is governed by an equation $f \sim \partial_q S(q)/S(q)$, where $S(q)$ is the cross-section area, and $q$ is the domain wall position. The gradient of the nanostripe cross section can become a self-driving force, that provides domain wall automotion similarly to the nanostripe curvature gradient. However, the variations of the cross section also introduce a Walker-like speed limit on a domain wall. For both of the showcased geometries we derive the asymptotic values of the domain wall velocity and values of cross section-induced Walker threshold including the curvature-induced corrections. In the straight nanostripe case the asymptotic velocity is shown to equal $V_s = -2\alpha^{-1}\partial_q S(q)/S(q)$, where α is the Gilbert damping coefficient. In the circle arc the asymptotic velocity reads $V_\varkappa \approx V_s (1 - \varkappa\Delta_0\pi/2)$, where $\varkappa$ is a dimensionless curvature, $\Delta_0 = 1/\sqrt{kT}$ is the domain wall equilibrium width, with kT being the easy-tangential anisotropy coefficient. All analytical predictions in this study are confirmed by the NMAG micromagnetic simulations [4].

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# Statics and Dynamics of Bimerons in Magnetic Topological Materials

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**Abstract ID #NMM-1247**

I will discuss topological magnetic textures, such as skyrmions, half-skyrmions (merons), and bimerons, which constitute tiny whirls in the magnetic order. They are promising candidates as information carriers for next generation electronics, as they can be efficiently propelled at very high velocities employing current-induced spin torques [1]. First, I will talk about bimerons [2, 3] in ferromagnetic systems coupled to heavy metals and topological materials. Then I will show that antiferromagnets can also host a variety of these textures, which have gained significant attention because of their potential for terahertz dynamics, deflection free motion [4], and improved size scaling due to the absence of stray fields. Finally, I will demonstrate that topological spin textures, merons and antimerons, can be generated at room temperature and reversibly moved using electrical pulses in thin film CuMnAs, a semimetallic antiferromagnet that is a test-bed system for spintronic applications [5].

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# New Opportunities for Spintronic Technology from Internet of Things to co-Processors

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**Abstract ID #NMM-1289**

The development of more efficient and high performance spintronic devices and the efforts to have co-integration of spintronics with CMOS technology is driving the development of hybrid CMOS-spintronic solutions for application where one can take the advantages of both technologies while minimizing their disadvantages. In this talk, I will focus on our recent developments on new potential applications of magnetic tunnel junctions (MTJs) as compact sensors for IoT nodes and computing applications. I will discuss how MTJs can be used to develop compact and more effective accelerometers and physical unclonable functions for security applications. I will also discuss our recent results on spintronic microwave amplifiers which are based on the phenomenon of injection locking. In this first part of the talk, I will discuss about a single MTJ spinking neuron which does not need any reset mechanism after the spike and it is equivalent in term of behaviour to what described by the Hodgkin-Huxley model.

In the second part of the talk I will focus on probabilistic computing with probabilistic-bits (p-bits) which is emerging as a computational paradigm able to be competitive in solving NP- hard combinatorial problems. I will show how to map hard combinatorial optimization problems (Max-Sat, Max-Cut, Traveling Salesman problem) into probabilistic Ising machine by using the idea if invertible logic gates and more complex energy mapping approaches and how to implement those in spintronic and CMOS technology. We will investigate the potential of advanced annealing schemes comparing simulated annealing, parallel-tempering, and simulated-quantum-annealing and how it will be possible to implement an efficient probabilistic co-processor.

**ACKNOWLEDGMENTS**

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# Thermally Generated Spin Transport and Spin Seebeck Effect in Thin Film Heterostructures

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**Abstract ID #NMM-1299**

Spin-heat coupling and thermo-spin transport are topical areas of interest for the spintronics community. The origin of longitudinal Spin Seebeck effect (LSSE) and its relationship with magnetic anisotropy as well as magnon propagation across magnetic insulator/heavy metal interfaces have remained challenging issues. LSSE induces incoherent magnon excitations with the application of a temperature gradient across the thickness of a magnetic material. Although the ferrimagnetic insulator $Y_3Fe_5O_{12}$ (YIG) is known as the benchmark system for LSSE, other members of the insulating rare earth iron garnet family, e.g. the compensated ferrimagnet $Gd_3Fe_5O_{12}$ (GdIG), ferrimagnet insulator $Tm_3Fe_5O_{12}$ (TmIG) etc., are of interest and have received less attention from the point of view of spin-caloritronics. We have pioneered the technique of RF transverse susceptibility to probe the effective magnetic anisotropy in magnetic materials and heterostructures. Combining the RF transverse susceptibility with LSSE measurements, we have shown correlation between bulk and surface anisotropy with the field and temperature dependence of LSSE in YIG/Pt heterostructures and other compensated ferrimagnets [1]. Recently, our group has shown, for the first time, a scaling of LSSE in GdIG/Pt bilayers with different thickness and on different substrates across the compensation temperature [2]. Our work on TmIG/Pt heterostructures with varying film thickness reveals the clear role of anisotropy and Gilbert damping on the LSSE [3]. From RF susceptibility, LSSE and broadband FMR experiments, quantitative analysis of the magnon propagation length and its correlation with magnetic anisotropy and Gilbert damping has been done. Overall, this talk would present new results in the thermal spin transport of garnet heterostructures which are of fundamental importance in spintronic.

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# Spin-Orbit Torque Sensors with Offset Cancellation for 3D field measurements

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**Abstract ID #NMM-1300**

Spin-Orbit Torque (SOT) sensors have garnered significant attention in recent years due to their potential for high sensitivity and low zero field offset [1,2,3] . This work provides a comprehensive overview of recent advancements in SOT sensors, focusing on key aspects including operational principles and active offset (zero field error) compensation.

This work delves into the latest developments in SOT sensor applications, encompassing magnetic field detection with active offset compensation and high sensitivity readout. In this study, we present a device designed for measuring magnetic fields below 1 mT with high sensitive readout in all 3 directions, while also compensating for offset in all three dimensions by spinning current techniques [4] and SOT modulations of the magnetization [3]. Furthermore the concept of a combined TMR Hall effect sensor, utilizing SOT, will be introduced. This combines the high sensitive TMR readout of Hall based devices, which allows for the cancellation of the zero field error.

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# Quantum Oscillation of Gilbert Damping in Ultrathin Fe Films

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**Abstract ID #NMM-1301**

We report thickness-dependent oscillations in the Gilbert damping of single-crystal Fe(001) films at low temperature due to discrete quantum well states of the $\Delta_5{}^{\uparrow}$ bands. The measured damping os- cillations are quantitatively reproduced by the torque-correlation model based on the first-principles band structure of Fe films. The band-resolved analysis suggests that Gilbert damping of Fe is dom- inated by the $\Delta_5{}^{\uparrow}$ bands due to strong orbital hybridization and shall not be measured by the total density of states. The dominant role of the $\Delta_5{}^{\uparrow}$ bands explains the recently reported ultralow damp- ing of FeCo and FeAl alloys. Our findings pave the way of controlling the damping parameter through shifting the relevant energy bands by doping or gating.

# Spin Wave Amplification Through Superradiance

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**Abstract ID #NMM-1305**

Superradiance is a phenomenon of multiple facets that occurs in classical and quantum physics under extreme conditions. Here we present its manifestation in spin waves under an easily realized condition. We show that an interface between a current-free (normal) ferromagnetic (FM) region and a current-flow (pumped) FM region can be a spin wave super-mirror whose reflection coefficient is larger than 1. The super-reflection is the consequence of current-induced spectrum inversion where phase and group velocities of spin waves are in the opposite directions. An incident spin wave activates a backward propagating refractive wave inside pumped FM region. The refractive spin wave re-enters the normal FM region to constructively interfere with the reflective wave. It appears that the pumped FM region coherently emits reflective waves, leading to a super-reflection. The process resembles superradiance of a spinning black hole through the Hawking radiation process, or Dicke superradiance of cavity photons inside population inverted media.

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# Fast Excitation Dynamics in Artificial Spin Ice

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**Abstract ID #NMM-1309**

Artificial Spin Ice (ASI) consists of magnetostatically coupled nanomagnets where frustration leads to multiple low energy states and propagating excitations [1]. These excitations, or emergent magnetic monopoles, are due to fictitious magnetic charges with a non-zero sum at the nodes between nanomagnets. Here the ASI is formed from the free layers of magnetic tunnel junctions (MTJs), which have faster dynamics than the larger patterns of traditional ASI, and offer the potential to inject excitations on one side of the array using spin transfer torque, and detect them on the other side via tunnel magnetoresistance (TMR). The free layers of the CoFeB-based MTJs are patterned into square arrays of 60 nm circular nanomagnets with a 90 nm pitch. A 7 Oe fringe field from the pinned synthetic antiferromagnet (SAF) reference layer breaks symmetry. Conductive atomic force microscopy of individual MTJs reveals a pattern of alternating easy axis directions, like that seen with larger ASI nanomagnets. Time-dependent TMR depends on the angle between the SAF field and the easy axis. If parallel there is zero field telegraphing between $\theta = 0$ and 180°, but if perpendicular there is significant spin canting relative to an average angle of 90°. Changes in the effective energy barrier are used to identify whether a particular nanomagnet is part of an emergent magnetic monopole excitation. Non-trivial propagation through the frustrated lattice, necessary for neuromorphic computing, has been achieved by applying an external field diagonal to the square ice pattern [2]. Here a rotated SAF field [3], relative to the ASI orientation, is used to favor a general propagation direction while allowing for non-linear response when excitations interact.

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# Delocalized Spin States At Graphene Nanoribbon Termini

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**Abstract ID #NMM-1330**

Magnetically active graphene nanoribbons (GNRs) have gained considerable research interest due to their potential applications in topological spintronic devices. However, GNRs are usually passivated during the synthesis process which leads to quenching of magnetic states. Here, we find magnetism can be revived through a post annealing process, where unpassivated atoms are located near the termini. Namely, a pair of intense Kondo resonances emerges at zigzag terminus, of 7-armchair GNR on Au(111), revealing the many-body screening effects of local magnetic moments. Although the Kondo resonance originates from a missing local orbital, it extends to a distance of 2.5 nm along the edge of GNR. The results are complemented by density functional theory calculations which suggest a possible coupling between Kondo states despite screening effects of substrate electrons. These findings highlight a possibility of inducing magnetic ordering in passivated GNR by de-hydrogenation of atoms at the peripheries of zigzag termini.

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# Magnetization Dynamics Fom Micro to Macro Scales: From Magnetic Rogue Waves to Macroscopic Artificial Spin Ice

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**Abstract ID #NMM-1334**

For hundreds of years, seafarers have told stories about enormous waves that appear out of nowhere and sink ships, but the physics of these rogue waves has only recently begun to be understood. Rogue waves are localized in time and space with amplitudes much larger than surrounding waves. Water rogue waves were relatively recently recreated with a time-reversal process, involving recording a localized pulse and re-emitting the time-reversed recorded waveforms, which interfere and refocus into a rogue wave [1]. Creating rogue waves in a magnetic environment poses an intriguing task since the time-reversal symmetry of the system is broken due to the fixed chirality of the precession of the magnetization vector and the presence of relatively large damping. Recently, this phenomenon has been demonstrated by micromagnetic simulations [2]. Here, I will present the first experimental observation of Magnetic Rogue Waves (MRWs). The measurements were performed using the near-field microwave scanning microscope technique in an out-of-plane-magnetized macroscopic thin film of Yttrium Iron Garnet (YIG) using a similar record-playback approach. The obtained results indicate strong localization of the MRWs even with a limited amount of four emitters used. We argue that these results would pave the way for the on-demand steering of large amplitude nonlinear spin waves in future magnonic computing devices.

Nonlinear effects in magnetic systems are not only limited to magnetic nano-elements. Artificial spin ices (ASIs) are ensembles of geometrically structured, interacting magnetic nano-elements that exhibit frustration [3]. In this talk, I will present a macroscopic ASI where 1-inch magnets mounted on low-friction rotors are arranged in a square lattice. The system is driven into a nonlinear regime by an external coil with a field of 2-20 Hz range. Mixing and coupling between high-symmetry modes is observed. The dynamics was experimentally captured by a high-frame-rate camera and then digitized to recover the spectrum for each magnet. Modeling based on the torque equation for each magnet and their coupling using a monopole-charge approximation [4] reproduces the dynamics with remarkable accuracy. While at completely different spatial and temporal scales, these dynamics are similar to those observed at the nanoscale ASIs [5]. Our macroscopic ASI can be considered as a testbed for nonlinear phenomena at a scale appropriate for dissemination to the general public. Moreover, we propose a similar design for the development of nanoscopic highly nonlinear magnetic systems.

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# Skyrmion Dynamics and Spin Wave Fractals Measured with in-situ SANS and SAXS

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**Abstract ID #NMM-1335**

Magnetic skyrmions are topologically protected chiral structures which have interesting fundamental qualities as-well as promise for magnetic data storage and logic technologies. One of the unique features of magnetic skyrmions is their well defined dynamic modes, including gyration and breathing modes. In this presentation I will highlight our recent works investigating the dynamic behavior of hybrid skyrmions in Gd/Fe multilayers.[1-3] This system is particularly promising because of its ability to sustain skyrmions at ambient conditions (room temperature and zero field) making them relevant for technological applications. The stability of this system is attributable to the skyrmions hybrid structure, which can be described as a stacking of three skyrmions (Neel-Bloch-Neel);[2] this structure reduces the magnetostatic energy in the system. Each of the regions of the hybrid skyrmion respond uniquely under dynamic gyration and emit a unique selection of spin waves. Magnetic dynamics are conventionally investigated using ferromagnetic resonance (FMR) spectroscopy, as is done here, to identify a field/frequency resonant condition. We then perform FMR while in-situ measuring the magnetic scattering using small angle neutron and X-ray scattering (SANS/SAXS). This approach allows us to determine the structure of the skyrmions, skyrmion lattice and the emitted spin waves during the dynamic gyration. For small excitations[4] the skyrmion lattice is largely insensitive to the dynamics, however the spin wave emissions are readily observable. Furthermore, the interference between these spin waves form a fractal network that is captured in the SANS pattern, allowing a direct measurement of the structure of the dynamic magnetic feature. Using a stronger excitation field, the scattering pattern acutely changes from a hexagon with flanking higher-order peaks to a hexagon, to simply two peaks. This denotes a transformation in the skyrmion from a structure akin to a pillar - with a thin domain wall - to a structure with a wider boundary, more similar to skyrmions in conventional non-centrosymmetric systems. The collapse in the intensity and resolution to two peaks identifies the skyrmion lattice collapsing. The results offer new insights into skyrmions, and more generally magnetic dynamics, offering a technique which may allow us a generalized approach to measure the structure of dynamic magnetic behavior.

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# Magnetic Relaxation Characteristic and Cancer Cell Suppression Effect of Magnetic Nanoparticles

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**Abstract ID #NMM-1337**

Nano-sized magnetic particles exhibit interesting phenomena, where that slight differences in particle size can significantly change the magnetic relaxation properties [1]. We provided magnetic nanoparticles of various compositions and particle sizes, focused on their AC magunetic susceptibility, and discussed the mechanism of magnetic relaxation. The magnetic particles were prepared by a wet-chemical method [2], and their local structures were analyzed by XRD and synchrotron XAFS measurements.

The imaginary part χ" of the AC magnetic susceptibility, i.e., the component lagging 90 degrees relative to the external magnetic field, is responsible for the heat generation in an AC magnetic field. Analysis of heat dissipation properties showed that in Ni-ferrite, Néel relaxation was dominant for particle sizes below 20 nm, and Brownian relaxation was dominant for larger sizes. The specific absorption rate calculation also predicts that large heat generation occurs at particle sizes of 13-17 nm.

Using this heat dissipation property, a study of cancer cells to which an AC magnetic field of 14.3 kHz, 17.2 kOe was applied for 30 minutes showed a significant cancer cell suppression effect. Interestingly, cancer cells were further killed after 24 hours of incubation after the AC magnetic field was turned off. On the other hand, cells that were not subjected to the magnetic field recovered. This suggests that hyperthermia treatment may cause an immune effect. The mechanism of cell death and heat-related proteins will be also discussed.

These magnetic nanoparticles also function as contrast agents for MRI and MPI [3], which could lead to a future application of "theranostics" that simultaneously performs treatment and diagnosis.

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# Synthesis of Fe-Based New Magnets

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**Abstract ID #NMM-1352**

Demand for high-performance magnet materials is increasing in various fields, including the automotive, electronics, and medical industries. However, the current mainstream permanent magnet materials contain rare earths and are faced with the problems of resource depletion and price escalation. Therefore, there is a need for new permanent magnet materials that do not contain rare earths. Particularly, materials with the CuAu crystal lattice structure ($L1_0$) have large uniaxial magnetic anisotropy, thus many studies on $L1_0$ type materials have been reported. However, it is a crucial problem that typical $L1_0$ type materials such as FePt, CoPt, and FePd include noble metals of Pt or Pd. To solve this problem, the development of novel magnetically anisotropic materials without noble metals is now eagerly expected. In this study, we aim to synthesize an $L1_0$ type FeNi alloy with a large magnetic anisotropy[1-4], which exists only in an iron meteorite as a Widmannstätten structure in nature. Single-phase $L1_0$ type FeNi powders were fabricated through a new chemical method, nitrogen insertion and topotactic extraction (NITE) [5]. In the method, FeNiN, which has the same ordered arrangement as $L1_0$ type FeNi, is formed by nitriding A1-FeNi powder with ammonia gas. Subsequently, FeNiN is denitrided by topotactic reaction to derive single-phase $L1_0$-FeNi with a chemical order parameter of 0.71. The transformation of disordered phase-FeNi into the $L1_0$ phase increased the coercive force from 14.5 kA/m to 142 kA/m, and an actual motor was fabricated. The proposed method not only significantly accelerates the development of magnets using $L1_0$-FeNi but also offers a new synthesis route to obtain ordered alloys in non-equilibrium states. We hope that, in the future, the NITE method will be developed further to facilitate the derivation of completely new ordered alloys that are superior in terms of characteristics such as magnetism, toughness, and catalytic performance.

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# X-ray Imaging Of Antiferromagnetic Dynamics

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**Abstract ID #NMM-1362**

Magnetic oscillations (magnons) are the collective excitations of ordered spin systems. Also referred to as spin waves, they are considered as low-loss information carrier for future highly-integrated signal and data processing devices.

Spin waves in ferromagnetic materials typically exhibit precession frequencies in the GHz or lower 10 GHz range. In general, the processing speed of a device directly scales with its frequency bandwidth. Therefore, systems with higher intrinsic precession frequencies are desired. In that respect, antiferromagnetic materials were found to exhibit precession frequencies up to the THz range. At the same time, it is demanding to probe antiferromagnetic systems, both statically and dynamically, as a result of their vanishing net magnetization in equilibrium. In particular, the nanoscale imaging of antiferromagnetic spin dynamics remained as a significant challenge.

In this contribution, we will present initial results from imaging single-crystalline, antiferromagnetic hematite ($Fe_2O_3$) by means of time-resolved scanning transmission x-ray microscopy (TR-STXM) [4], employing both x-ray magnetic linear and circular dichroism (XMLD/XMCD) as contrast mechanisms [5]. In the canted antiferromagnetic state at room temperature, we observe coherent spin waves in the frequency range from approximately 15 GHz to 40 GHz, and at group velocities of the order of 20 km/s. These results will contribute to the general understanding of real space antiferromagnetic dynamics.

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# Spintronics for Massive Data Memory-Storage – Past, Present and Future

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**Abstract ID #NMM-1368**

Spintronics is a field of research that harnesses the electron's spin to create novel materials with exotic properties and devices especially those for storing digital data that is the lifeblood of many of the most valuable companies today. Spintronics has already had two major technological successes with the invention and application of spin-valve magnetic field sensors that allowed for more than a thousand-fold increase in the storage capacity of magnetic disk drives that store ~70% of all digital data today. Just recently, after almost a 25-year exploration and development period, a high performance nonvolatile Magnetic Random Access Memory, that uses magnetic tunnel junction memory elements, became commercially available. A novel spintronics memory-storage technology, Magnetic Racetrack Memory is on track to become the third major success of spintronics. Racetrack Memory is a non-volatile memory in which data is encoded in mobile chiral domain walls that are moved at high speeds by spin currents to and thro along synthetic antiferromagnetic racetracks. In this lecture I will introduce the basic physics and especially the novel atomically-engineered materials that make possible these three spintronic technologies.

TRACK 9

# “SUPERCONDUCTIVITY IN NANOSCALE & MESOSCOPIC SYSTEMS”

# New Topological Transitions in Superconductor 3D Nanoarchitectures

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**Abstract ID #NMM-0949**

Advanced high-tech fabrication techniques include a chemical synthesis of nanotubes, a physical Glancing Angle Deposition technique, strain-driven roll-up self-organization, direct-writing approaches using focused ion- or electron-beam induced deposition, automated design of scaffolds from 3D DNA-based origami. These pathways made it possible to fabricate geometrically complex and topologically nontrivial 3D nanoarchitectures, which reveal novel electronic, magnetic, optical and transport properties [1]. In 3D superconductor nanoarchitectures, a topological transition between the vortex and phase-slip regimes determines the magnetic-field-voltage and current-voltage characteristics revealing a nontrivial topology of SC screening currents. An abrupt switch-on of the transport current triggers the transition from the vortex- to phase-slip-regime in superconductor open nanotubes [2]. Various dynamic topological transitions in superconductor open nanotubes take place under a combined dc+ac transport current [3]. Recently, microwave generation by vortex jets in superconductor nanotubes [4] and symmetry breaking by tilted fields [5] have been explored. Relying upon the time-dependent Ginzburg-Landau equation, it is found that vortex chains, vortex jets, and phase-slip regimes occur in superconductor open nanotubes due to the inhomogeneity of the normal magnetic field component. Distinct from planar thin films, the vortex jets are constrained within the half-tubes and correlate strongly between them. At lower magnetic fields, vortices follow the same path within the half-tubes, forming single vortex chains. At higher magnetic fields, the vortex trajectories undergo multifurcations, giving rise to patterns composed of vortex jets consisting of two or more vortex chains. Due to a stronger confinement of single vortex chains in tubes of small radii, jumps in the average voltage and frequency of microwave generation are unveiled, which occur when the number of fluxons moving in the half-tubes increases by one [4]. The peaks in the induced voltage and jumps in the microwave generation frequency as a function of the applied magnetic field are predicted for nanotubes of rather small radii pointing to the decisive role of the interaction of vortices in the both half-tubes for the correlated vortex dynamics. Effective steering of vortex chains and jets is realized by tilting the magnetic field in the plane perpendicular to the nanotube axis, with a jet-to-chain transition unseen for planar constrictions [5]. In addition to prospects for the tuning of GHz-frequency spectra and the steering of vortices as information bits, the discussed findings lay the foundation for on-demand tuning of vortex arrangements in superconductor 3D nanoarchitectures in tilted magnetic fields.

## ACKNOWLEDGMENTS

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# Nanoscale Room-Temperature Superconductivity in Biological Systems

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**Abstract ID #SNMS-0955**

Superconductivity is basic quantum-mechanical phenomenon with multiple technological applications, among which is quantum computing [1]. It is usually associated with metals and low temperatures but theoretically was extended to room temperature, organic, and biological materials [2,3]. For room-temperature superconductivity, an unconventional mechanism is needed, preferably in a system with reduced dimensionality. The experimental attempts in search for such superconductivity are under the way. Here the experiments with microtubules, nanometer-scale quasi one-dimensional structures abundant in the brain are presented arguing that they are in the superconducting state at the room temperature. Complementing already published data on electrical transport [4] and magnetic [5] measurements, this research focuses on magnetic flux quantization and Josephson radiation coming from the connections of microtubules in the neurons during the propagation of action potential. A mechanism for such generation is suggested. It is argued that nanoscale superconductivity is responsible for quantum processing of information in the microtubules, while coherent Josephson radiation helps synchronizing functions of living organisms. To put idea of the room temperature superconductivity on a solid basis, the values of its main parameters like energy gap, critical temperature, magnetic penetration depth, and coherence length are estimated. The results could improve understanding of quantum-mechanical basis of the biological systems in a humid and warm environment arguing that nanoscale room-temperature superconductivity perfectly survives in this environment and plays important role in the functioning of living organisms.

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# Vortex Jets in 2D and 3D Superconductor Nanomembranes

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The dynamics of magnetic flux quanta (Abrikosov vortices) determine the resistive response of superconductors. In pinning-free 2D thin films, the penetration and motion of vortices are controlled by edge defects, leading to such arrangements as vortex chains, vortex jets, and phase-slip regimes. Previously, we shown theoretically and experimentally [1] that at sufficiently large transport currents, a defect at the edge of a superconducting strip can act as a gate for the vortices entering into it. These vortices form a jet, which is narrow near the defect and expands due to the repulsion of vortices as they move to the opposite edge of the strip, giving rise to a transverse voltage. The one-by-one penetration of vortices leads to the appearance of kinks in the current-voltage curve, whose presense therefore can be used for fluxon counting and velocimetry [2].

In our recent work [3], relying upon the time-dependent Ginzburg-Landau equation, we have predicted that vortex jets should appear in 3D superconductor open nanotubes even without edge defects, due to the inhomogeneity of the normal magnetic induction component Bn, caused by the 3D tube geometry. In contrast to 2D thin films, the vortex jets in 3D open tubes are not diverging because of constraint to the tube areas where Bn is close to maximum. Furthermore, by tilting the direction of the applied magnetic field an angle α in the plane perpendicular to the axis of a nanotube carrying an azimuthal transport current, it is possible to steer vortex chains and vortex jets to a given point of the sample [4]. This approach surpasses the capabilities of vortex guiding in nanoengineered pinning landscapes in terms of reconfigurability.

In all, our findings are essential for novel 2D and 3D fluxonic devices which can operate in few-and multifluxon regimes.

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# Ising Superconductivity and Anisotropy in Noncentrosymmetric Quasi-2D Systems

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**Abstract ID #SNMS-1296**

New type of superconducting interaction – the Ising pairing – has been discovered in the atomically thin $NbSe_2$ [1]. The lack of crystal inversion symmetry in 1*H* monolayer combined with a strong spin-orbit coupling leads to an effective spin-orbit magnetic field which locks spins in the Cooper pairs out of plane and hinders the spin pair-breaking. This leads to anomalously high in-plane upper critical field strongly violating the Pauli limit. Adding layers to 1*H*-$NbSe_2$ rapidly suppresses Ising superconductivity due to restoration of the inversion symmetry but we have shown that bulk misfit layer systems $(LaSe)_{1.14}(NbSe_2)$ and $(LaSe)_{1.14}(NbSe_2)_2$, superconductors with $T_c$ = 1.23 K and 5.7 K, respectively reveal a huge in-plane upper critical field exceeding the Pauli limit even more that in $NbSe_2$ monolayer [2,3]. The misfits are highly anisotropic as they comprise incommensurate $NbSe_2$ and LaSe layers. Utilizing both experimental and theoretical means we show that our systems are electronically equivalent to the highly doped $NbSe_2$ monolayer breaking the inversion symmetry in the crystal [4]. Recently, we show that in a 4*H* polyform of notoriously studied single crystalline $NbSe_2$ with $T_c$ = 6 K which is much less anisotropic than the misfits, the huge upper critical field above 25 T is also of Ising origin.

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TRACK 10

# “NANOSENSORS, NANODEVICES & APPLICATIONS”

# Advancements in Robust Planar-Hall Magnetoresistive Sensors for On-Demand Applications

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**Abstract ID #NNA-0941**

Recent advancements in micro- and nanotechnology have led to the widespread use of spintronics sensors, particularly in recording and non-recording applications. Notably, Planar-Hall magnetoresistive (PHMR) sensors stand out in this technology, offering exceptional sensitivity and ultra-low field detectivity. Their versatility makes them suitable across various industries, including the Internet of Things, mobile devices, space technologies, aeronautics, magnetic flux leakage detection, environmental monitoring, and healthcare. [1,2].

This study provides a comprehensive review of PHMR sensors, emphasizing their high thermal stability and tunable field sensitivity. Here, thermal drift is very low about 0.02 Ω/°C, compared to other MR sensors, which is around 10 Ω/°C. Another aspect involves the tunable field sensitivity, ranging from approximately a few μV/Oe for the cross-type configuration to 2 mV/Oe for the 7-ring sensor. This sensitivity is achieved through adjustments in the exchange coupling field by inserting a nonmagnetic Cu layer between NiFe and IrMn and varying the number of rings in the sensor. [3]. Furthermore, utilizing high resistive material (Ta, W) as a seed layer increases the output signal and sensitivity by 20% and 5%, respectively, by improving the crystallinity of the sensing layer.

Due to their robust nature, PHMR sensors can be deployed in many applications, including those in harsh environments and those that require high-accuracy measurements, such as lab-on-chip magnetometries integrated with micro-fluidic channels for biochips, flexible sensors, and industrial modules. [4]. These applications showcase the remarkable sensitivity of PHMR sensors, with a maximum magnetic moment resolution of ~ $10^{-14}$ emu in dried conditions, which are $10^4$ orders of magnitude better than conventional SQUID magnetometers [5]. With their ability to be customized and miniaturized and their cost-effective nature, PHMR sensors are uniquely competitive and offer significant potential for mass production and non-recording industrial applications.

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# Study on the Optical and Gas Sensing Properties of Eu-doped ZnO

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In this work, Eu-doped ZnO columnar films were prepared with SCS (chemical synthesis from solution) approach, with different doping concentrations, noted as Eu2 (0.1 at% Eu) and Eu4 (0.2 at% Eu). The morphological and optical properties were analyzed using SEM (Scanning electron microscopy), transmittance spectra, and responsivity spectra. It was observed that Eu doping concentration does not change morphology significantly, but slightly influences the size of the columnar grains. By increasing the Eu doping concentration, a decrease in transmission can be seen, which was also confirmed by responsivity spectra, revealing higher responsivity for Eu4 than the Eu2 sample. Due to the shallower penetration depth of shorter wavelengths, higher responsivity can be observed for 280 nm UV illumination than other higher wavelengths. The gas sensing properties have been studied for the Eu2 sample which shows a good response towards 100 ppm H2, VOC gases at 300 ℃. The UV sensing properties of columnar films were investigated and the results revealed that higher Eu doping concentration significantly enhances the optical properties.

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# Back-Gated Field-Effect Transistors with 2D Materials and Their Heterojunctions

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**Abstract ID #NNA-1026**

Two-dimensional (2D) materials, along with their van der Waals heterojunctions, hold immense promise for electronic and optoelectronic applications.

In this presentation, we delve into several critical aspects related to electrical transport and photoconduction within 2D materials, specifically focusing on black phosphorus (BP) and transition metal dichalcogenides like MoS2 and ReS2.

We investigate back-gate transistors with channels composed of either a single material or a heterojunction of two materials (e.g., BP/MoS2). These studies are conducted under varying air pressures and temperatures, both in darkness and under illumination. The dominant n- or p-type conduction and the observed rectification of the devices can be understood through an energy band model that considers the van der Waals heterojunction together with the interfaces that the 2D materials form with the metal contacts.

Our findings reveal that temperature and air pressure significantly influence both electrical conductivity and photoconductivity. Photocurrent transient measurements highlight the dominance of slow photobolometric and even slower photogating effects in the photoresponse of 2D materials-based devices.

Temperature and light-induced desorption of adsorbates, such as O2 and H2O molecules, and photogating effect due to charge trapping contribute to the occurrence of positive and negative photoconductivity in the same device. These phenomena are gaining attention due to their potential for fabricating multifunctional devices, that can serve as memory elements or find applications in neuromorphic vision sensors.

In summary, this presentation sheds light on some intriguing properties of 2D materials and their potential for applications in the field of electronics and photonics.

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# The p-n Heterostructured Thin Films for Ultra-sensitive Methane Gas Sensors

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**Abstract ID #NNA-1072**

Methane are highly explosive at concentrations of about ~ 5% in air, it makes the leak detection very important [1]. The main sources of methane are coal, peat deposits, and methane is also associated gas in the extraction of hydrocarbons [1]. Unfortunately, 180 people have died only over the past 30 years in the Republic of Kazakhstan in mines mainly caused by the explosion/emission of methane, including 172 people in the coal mines of the Karaganda region [2]. The recent accidents occurred at the Abayskaya mine on 07.11.2021 , where 6 people died [2] and Kostenko mine where 45 people died, the preliminary caused by methane gas explosion [3]. The one of the most tragic accident in the CIS was at the Listvyazhnaya mine on November 26, 2021, where 54 people died. The accidents were caused by a sudden release of methane and the ensuing explosion, and consequent a coal dust fire [4]. Of course, improving safety is the cornerstone of preventing such accidents. Predicting possible methane emissions from coal seams (drifts) is one of the methods for solving the existing problem.

The conductometric detection method is the most promising for gas sensing since it provides the possibility to detect at deficient concentrations (<1ppm) with quick response (<30s). The chemo-resistive sensors are considered compact, robust, with versatile applications, and low cost, and could be an equally efficient alternative for broad use in gas monitoring systems. One of the types of chemo-resistive sensors is the metal oxide semiconductor (MOS) sensor. The MOS sensor's working principle is based on reversible chemisorption of reducing gases (H2, CH4) or oxidizing gases (O2, NO) on the sensing material surface. These processes cause reversible changes in its conductivity [5]. Oxygen molecules in the air adsorb onto the sensor surface, which leads to the appearance of a depletion layer and a decrease in the conduction band, respectively. It is known that the adsorbed oxygen on the sensor surface exists in three different forms ( , , and ) [6], and their distribution heavily depend on the operating temperature [7]. The deposited oxygen ions on the sensor surface react with the molecules of the reducing gas and lower the potential barrier and increase conductivity, while for oxidizing gas, it works vice versa.

The research work aims development of an gas monitoring device that utilizes p-n junction heterostructured nanorods made from a combination of MOS (Fe2O3 /TiO2). This device demonstrates exceptional specificity for methane gas and exhibits a very high sensitivity at room temperature. Our simulations will provide a deeper understanding of how p-n junction heterostructured nanorods made from MOS (Fe2O3 /TiO2) interact with CH4.

## ACKNOWLEDGMENTS

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# Biowaste-derived Carbon Dots and Metal Organic Frameworks Heterostructures-based Printable Biosensors

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**Abstract ID #NNA-1073**

A biosensor generates interpretable signals proportional to the concentration of an analyte, thereby identifying biological or chemical processes. The applications of biosensors are diverse, spanning disease monitoring (e.g., for COVID-19), drug research, and detecting contaminants and pathogens in bodily fluids like blood, urine, saliva, and sweat [1]. Notably, electrochemical biosensors dominate 80% of the market due to their wide-ranging applications in healthcare and environmental monitoring. And by combining this sensing technologies with nanomaterials possessing various dimensionalities, high surface-to-volume ratios, and strong conductivities, challenges related to sensitivity, repeatability, and selectivity can be effectively addressed.

In the pursuit of converting waste into valuable resources, we have synthesized carbon dots (CDs) from citrus peels, endowed with out-of-plane functionalities and covalent bridges to create porous and adjustable host structures known as Metal-Organic Frameworks (MOFs). We propose hybrid structures of BWCDs (bio-waste-derived CDs) and MOFs as an optimal base material to develop the detection platform for TNF-α, a pro-inflammatory cytokine crucial for early prognosis and treatment of numerous diseases, including Alzheimer's disease, sepsis, and cancer [2-4]. The developed material enables straightforward structural adjustments, including the arrangement of metal centers within MOFs, and the spatial distribution of BWCDs within MOF crystals, to facilitate antibody immobilization. The synthesized material undergoes effective characterization through techniques such as scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), and X-ray diffraction (XRD). Furthermore, utilizing this material as an ink for printing the biosensors, we explore a novel technique called scanning electrochemical microscopy, which allows for the detection of minute concentrations of the TNF-α by studying electrochemical reactions at a micro-scale dimension.

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# Spectroelectrochemical Characterization of Gold Nanoparticles and Polyaniline Composites and Their Application in Hydrogen Peroxide SERS Detection

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**Abstract ID #NNA-1080**

Surface-enhanced Raman scattering (SERS) allows for enormous enhancement of the Raman signal by placing the analyte on the surface of nanostructured plasmonic metals (Au, Ag, Cu). In recent years, works have been carried out in which plasmonic nanoparticles modified with electroactive compounds (including conductive polymers) were used in SERS research. Such compounds, by changing their structure in oxidation/reduction processes, are characterized by a changed Raman spectrum depending on the potential. SERS analysis of these processes allows for a better understanding of their molecular behaviour, detection of individual compounds (e.g. oxidants [1]), and even determination of the intracellular redox potential [2].

Polyaniline (PANI) is a conductive polymer characterized by high stability and a strong SERS spectrum. We used its composite with gold (Au) nanoparticles for electrochemical SERS studies. The obtained structures were electroactive at neutral pH, and their Raman spectrum changed significantly under the influence of different potential values. We checked the influence of the type of buffer and pH on the spectroelectrochemical properties of the Au@PANI composite. Then characterized it using voltammetry, UV-Vis spectroscopy, and TEM/EDS techniques. We decided to use the obtained nanocomposites to detect hydrogen peroxide ($H_2O_2$). Even though $H_2O_2$ is a strong oxidant, polyaniline on the gold surface began to oxidize at its relatively high concentration (about $10^{-4}$M). However, we observed that the addition of horseradish peroxidase (HRP) reduced the detection limit by several orders of magnitude.

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# Detection of Organic Molecules Using Modified Graphene Oxide and Gold Nanoparticles SERS Substrates

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**Abstract ID #NNA-1081**

Methods for detecting various chemicals are in constant development. Scientists try to develop methods that are as sensitive and simple as possible to use. Surface-enhanced Raman spectroscopy appears to be ideal for this purpose. To achieve the desired Raman signal enhancement, it is necessary to use appropriate substrates. Plasmonic metal nanoparticles or rough metal plates are often used. In recent years, interest in graphene oxide has increased as a good substrate material. It has been proven that it enhances the Raman signal of the analyte [1].

In this work, we present a combination of two enhancing effects: electrochemical - coming from gold nanoparticles - and chemical - coming from graphene oxide. Our previous work related to the conditioning of graphene oxide in various solutions has an impact on its spectroscopic properties [2].

Graphene oxide modified in solutions with pH = 1, 5.6 and 13 was used to create the substrates, as well as gold nanoparticles in the shape of nanobowls, which in previous studies showed very good enhancement of the Raman signal [3]. The tested organic molecules were rhodamine 6G and folic acid in the concentration range from $10^{-5}$ M to $10^{-12}$ M.

It has been proven that a composite consisting of graphene oxide modified in a solution at pH = 1 and gold nanobowls better enhances the Raman spectra of organic molecules compared to substrates with graphene oxide modified at a higher pH. Based on the collected spectra, a difference was also noticed in the method of adsorption of folic acid on the substrate surface. At low pH, it is adsorbed through the aromatic ring derived from p-aminobenzoic acid, while at higher pH values, folic acid is adsorbed randomly.

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# Photoluminescence Label-Free Biosensors: Current Trends and Perspectives

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**Abstract ID #NNA-1081**

The development of new approaches and methodologies for biosensor applications continues to be an active field of research. In recent years, the world has been challenged by pandemics (e.g., COVID-19), health issues, food security, and other biotechnology risks. In this regard, developing highly sensitive and stable technologies for detecting various bioanalytes (e.g., viruses, bacteria, toxins, etc.) is necessary. Biosensors are considered the most effective detectors because of their high sensitivity, selectivity, reproducibility, and stability.

Typical biosensors comprise a biorecognition element (antibody, DNA, enzyme etc.) and a transducer. The binding event, for instance, antibodies and antigens interaction) is transformed into a detectable signal of a transducer (e.g. optical, electrical, electrochemical, etc.) Depending on the transduction mechanism, biosensors are classified into several types, such as electrical, electrochemical, piezoelectric, thermal, and optical. Among different types of biosensors, optical biosensors become more attractive for end-users due to their small dimensions, lightweight, and portability. As a matter of fact, optical biosensors are currently considered to be the "gold standard" for the development of highly sensitive biosensors. Besides, the optical methods are non-destructive; these devices do not require electric contacts and demonstrate high precision in measurements. Thus, it makes the optical biosensors simple to use and low-cost.

Optical biosensors, in turn, may be classified into two groups depending on (i) the type of optical signal (reflectance, photoluminescence, absorbance, surface plasmon resonance, etc.) and (ii) label-based and/or label-free biosensors. The photoluminescence-based (PL) biosensor, which will be overviewed, is the most promising as it provides low cost and miniaturization of the biosensing elements (laser emitting diodes and optical fiber technique). A label-based sensing mode is based on the optical signal (colorimetric or luminescent) produced by some specific molecules (labels) attached to the analyte or its antibodies. However, this detection method may introduce systematic errors in the biosensing tests. Label-free biosensors enable the detection of biomolecular interactions in real-time without any fluorescence markers. The detected signal (e.g., changes in PL intensity, the shift of PL peak, etc.) for a label-free detection is generated directly by a transducer after the interaction between the analyte and the biorecognition element. The latter mode requires a lesser cost and expertise to develop effective biosensors.

We will demonstrate the fundamental principles and properties of the PL label-free biosensors. The role of nanotechnology in the fabrication of sensitive templates and transducers will be revealed. Future perspectives of PL-based label-free biosensors will be discussed.

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# Conducting Polymer - Titanium Dioxide Nanostructures for Toxic Gas Detection

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**Abstract ID #NNA-1084**

Currently, the rapid detection of toxic substances in areas contaminated by warfare or human activities is crucial. Essential for environmental monitoring are chemosensors that selectively react to a specific object and are used for qualitative or quantitative determination of the analyzed substance. The main issue in the operation of such sensors is the selection of an indicator substance responding to the action of chemicals by changing its physical properties [1]. Conducting polymers, particularly poly(o-toluidine) (PoT), are promising materials for the development of sensitive elements [2]. By incorporating inorganic clusters such as graphene, silica, metal oxide, etc. into the polymer shell, the sensitivity and selectivity of polymer sensors can be significantly improved. Previous research has demonstrated that the SiO2 introduction into the composites with polyaniline can enhance the temperature stability of such sensors. However, the sensory ability of organic-inorganic structures based on PoT with TiO2 nanoclusters has not been studied enough.

The hybrid organic-inorganic composites based on poly(o-toluidine) were prepared by both chemical and electrochemical "in situ" polymerization in the presence of TiO2 nanoparticles and toluene sulfonic acid (TSA) as a doping agent. TEM, SEM, and XRD analysis confirmed the formation of core-shell structures of prepared nanocomposites. We studied the influence of the toxic vapors (dimethylformamide (DMF), nitrobenzene (NB), toluene, tetrahydrofuran, etc.) on the specific resistance and optical absorption of new elements for gas sensing. The composites exhibit sensitivity of electrical resistance and optical absorption to organic solvent vapors. The character of this effect depends on the nature of the toxic substance. It was established that upon contact with vapors of DMF, the surface resistance of the PoT/TSA−TiO2 film increases by 1.5-1.6 times, reaching its maximum value in 500 seconds. The sensitivity, defined as the ratio of the change in resistance to the initial value, is 60%. While using nitrobenzene as a solvent, the specific resistance changes quickly but insignificantly, and the sensitivity does not exceed 4% (or 1.04 times). This type of resistance change is probably related to the possibility of the surface complexes formation between the composite nanoparticles and solvent molecules and may be used for their selective recognition. The changes in optical absorption spectra of the PoT/TSA-TiO2 films also prove enhancement in the sensitivity to toxic gases compared with unfilled polymer films.

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# Towards Nanosheet Field Effect Transistors

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**Abstract ID #NNA-1120**

The present paper addresses the late development of advanced CMOS technology starting from FinFETs to advanced (3D) technologies such as nanosheet FETs bridged by Gate All Arround GAAFETs. This development is pushed by the More than Moore's Law as need for rapid, small and low power (new) devices. Gate control has been improved from almost gate to all gate electrostatic control.

GAAFETs are characterized by the better electrostatic and reduced short channel effects, this made GAAFETs the promising devices for next generation of nanoelectronic Integrated Circuits. Hoever, it has been found that the effective channel width (Weff) to layout foot print (LFP) ratio is low causing smaller ION/IOFF ratio. Moreover, vertical layer stacking increased the parasitic capacitances and hence, drastically affected the device switching characteriscs.

Intorducing nanosheet transistors could eliminbate the GAAFET drawbacks. The main advantage of NS-FETs is their compatibility with other materials like Ge, SiGe and others.

In this work we will make a comparative study between the three FETs (FinFET, GAAFETs and NSFETs). As the NS FETs is considered to be a leading device of the semiconductor device industry in the next years, a simulation study related to its performances is made and basically it has been found that the characteristics are superior compared to other considered devices.

We have achieved simulations on different devices of 7nm gate length and showed that the Nanosheet FET in its different variant will help to stretch the Moore's Law for the next decades.

For better performance devices, nanofabrication 3D technology still needs more improvements. 3D integration technology is the today and future device and ICs fabrication tools. FinFETs will be gradually replaced by GAAFETs and later on by MBCFETs or NSFETs whicha are supposed to be be key elements in the next two decades. However, improvements in technology itself seem to be crucial.

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# Gate-All-Around Silicon Nanowire Field Effect Transistor Behavior at High Gate Voltages

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**Abstract ID #NNA-1131**

Gate-all-around field-effect transistors (GAAFETs) using a cylindrical silicon nanowire (SiNW) at its core are considered to be a preferable candidate for the future of the semiconductor industry and a promising successor to Si FinFET [1]. Some of the major advantages of silicon nanowire devices are their compatibility with current Si fabrication processes, their better channel electrostatics gate control, and their fewer parasitic components [2]. In order to fully understand the performance of GAAFET with silicon nanowires, it is important to study its detailed charge transport operation.

In this work, we report the result of such a study utilizing an electron transport model using Ensemble Monte Carlo (EMC) simulations coupled self-consistently with an electrostatic solver that solves Gauss Law in integral form. This modeling, even though computationally intensive, allows us to correlate the device behavior with the charge-carriers physics, including transport and scattering. Details of the EMC transport model, including band structure calculations, phonon dispersion, and electron-phonon scattering rates can be found in our earlier work [3,4]. The SiNW considered here as the active channel is [110] axially aligned. It has a diameter of 1.3 nm, and it is coaxially aligned with the GAAFET structure. The source and drain contacts are considered ideal Ohmic. The gate metal is considered ideal with no work function difference from the SiNW channel. The insulator considered is SiO2. The simulations are for the ambient temperature of 300 K. The simulation results suggest the observance of a negative differential resistance (NDR) in a gate-all-around field effect transistor (GAAFET) with a pseudo-1D small diameter SiNW as the active channel. This phenomenon is observed to occur at high gate voltages. While the exact cause of this is under investigation, it may be attributable to the decrease in the electric field along the channel. This causes the electric field along the channel to decrease and a large part of the channel to be nearly equipotential because of greater gate control. This in turn results in electrons moving with a lower velocity, and consequently lower drain currents. The increased Vgs (gate voltage) has a relatively smaller effect on increasing the number of channel electrons to compensate for the decreased electron velocity. This is because of the 1D nature of the channel, where the Columb repulsion from a channel electron strongly inhibits additional electrons from entering the channel.

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# Optical and Acoustic Surface Sensitive Techniques for Advanced Biosensing

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**Abstract ID #NNA-1176**

Optical and acoustic surface-sensitive methods are used to analyze and characterise surfaces with respect to their optical or acoustic properties. These techniques are applied in various fields, such as materials science, nanotechnology, biomedicine, and environmental science. Some of these methods can be combined during one measurement and provide different information such as physical, chemical, and mechanical properties of the same process measured in real time.

Quartz crystal microbalance with dissipation (QCM-D) is an acoustic method that is able to detect changes in quartz crystal frequency and dissipation caused by surface interactions and is used in chemical sensing and biosensing applications. The method of spectroscopic ellipsometry (SE) is an optical method that is able to measure changes in the polarisation state of light reflected from a surface to determine properties such as thickness and refractive index. Moreover, ellipsometry can be applied in combination with QCM-D and measure optical properties during the formation of biomolecules monolayer.

Despite that both of these methods are applied for biosensing purposes separately, the complementary application of both these methods for real-time biosensing is still rare. In the present work, we seek to demonstrate what possibilities of SE and QCM-D methods can be obtained during their application for biosensing. Moreover, we demonstrate the complementary application of these methods for the investigation of biomolecules monolayer formation. Our study demonstrates how these methods can provide information about immune complex formation at the solid-liquid interface in real-time.

We hope that the combination of these methods can provide broad-range information on monolayers formation at the solid-liquid interface not only for biomolecules but also for other nano-size objects as well.

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# Effect of Substrate on the Diffusion Process in Silver Nanowires

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Growing demand for transparent and flexible electronic devices in the world in recent decades has caused researchers to tend to optimize the electrical, mechanical, and optical properties of materials for these applications. One of the most useable kinds of materials in that field are metallic nanowires (NWs) and especially Ag NWs because of their special electric and physical properties. Optimization and achieving stable working conditions for NWs, especially Ag NWs are important to realize the great potential for NEMS, MEMS, and electronic applications [1]. For improving conductivity in NWs after synthesis the heat treatment process is pivotal. However, heat treatment can have a drastic effect on the morphology of NWs due to Rayleigh instability and energy minimization via spheroidization. This effect causes decreasing of conductivity at temperatures as low as 200-300 degrees Celsius. The dominant driving force for changing the morphology of NWs in sub-melting temperatures is surface diffusion. In Ag NWs with well-defined pentagonal cross-sections, one facet of the structure is in contact with the substrate, and other facets are free. This issue influences the diffusion dynamics and has a great impact on morphological changes in NWs [2]. In the current research, the effect of substrate on the surface energy and diffusion process causing fragmentation was studied at different temperatures. Structured Si substrates with holes were produced, and Ag NWs were deposited on these substrates resulting in either suspended (all five facets free) or adhered configuration (tight contact with Si substrate by one facet). Two different approaches were used in this study. First, with cycles of continuous heating and cooling and the other with one cycle of heat treatment at a chosen temperature. Different behaviors were seen in these schemes. In the first scheme, most of the NWs fragmented in the middle of the suspended part and in scheme two most of the suspended parts were preserved while the adhered parts were severely fragmented. The transmission electron microscopy results confirmed that fragmentation happens via diffusion without involving melting of NWs, there was no change in the atomic structure of NWs after heat-induced fragmentation. Also, we performed finite element methods and molecular dynamics simulations to compare with experimental results. Our findings provide insights into the effects of substrate and investigating the behavior of diffusion in nanowires that have suspended areas and non-suspended areas will be helpful in designing nanostructures for applications such as NEMS, MEMS, and flexible electronic.

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# Surface Functionalization of Upconverting Nanoparticles: Effect of Oligo(Ethylene Glycol) Substituent Length on Colloidal Stability and Cellular Uptake

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**Abstract ID #NNA-1197**

Nanoparticle surface modification is crucial for enhancing the stability of optically active nanoparticles in aqueous colloids and improving their biocompatibility and functionality. Modified particles may exhibit improved cellular uptake [1], prolonged circulation in the bloodstream, and enhanced membrane permeation [2]. However, materials used for modifying nanoparticles for biomedical applications must meet specific requirements: they should be non-toxic and exhibit good adhesion properties to firmly attach to the particle surface.

This study aimed to synthesize well-defined comb copolymers and utilize them for surface modification of upconverting nanoparticles for bioimaging purposes. Upconverting nanoparticles with a core-shell architecture and the general formula NaGdF4:Yb3+Er3+@NaGdF4:Yb3+Nd3+ were synthesized in our laboratory using a protocol described in our recent publication [3]. Polymers, with the general formula p(DMAm-co-OEGxMA), were synthesized via RAFT polymerization of DMAm (a non-commercial monomer synthesized in-house) and a monomer, OEGxMA, containing oligo(ethylene glycol) substituents of various lengths (where x represents the number of ethylene glycol repeating units). The properties of the synthesized polymers were evaluated using FTIR, NMR, and SEC techniques. These polymers were then employed for surface modification of upconverting nanoparticles to investigate the effect of oligo(ethylene glycol) substituent length on the stability and cellular uptake of the modified nanoparticles. Successful modification was confirmed by measuring the change in zeta potential of the nanoparticles in aqueous dispersion. Long-term stability of the nanoparticles in aqueous media (DI water at pH 6.2) and biological media (DMEM and DMEM supplemented with 10% FBS) was evaluated by measuring emission intensity over time. Subsequently, the upconverting nanoparticles modified with copolymers containing different lengths of oligo(ethylene glycol) substituents were transferred to the laboratories of the National Cancer Institute (Lithuania) for detailed accumulation studies in cancer cells with varying tumorigenicity (prostate C4-2, breast MDA-MB-231) and skin mesenchymal stem cells (S-MSCs). The latest results indicate that the upconverting nanoparticles are biocompatible and exhibit relatively high accumulation in cancer or mesenchymal cells and could be employed as biocompatible nanoprobes for bioimaging.

## ACKNOWLEDGMENTS

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# $WO_3$/ZnO NANOCOMPOSITE FOR ANTENNA APPLICATIONS

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**Abstract ID #NNA-1216**

An antenna is a passive electronic device that can both send and receive electromagnetic waves at a specific frequency range. The antennas used in today's communication systems need cutting-edge design and manufacturing techniques to provide high efficiency, great flexibility, and minimal radiation impact on the human body. $WO_3$ nanoparticles, ZnO nanoparticles and $WO_3$/ZnO nanocomposite were successfully synthesized by wet chemical method and studied as an antenna material. The effect of $WO_3$, ZnO and $WO_3$/ZnO nanocomposite on structural and morphological properties were studied systematically by using powder X-ray diffraction (XRD), scanning electron microscopy (SEM). The XRD studies which confirmed the presence of crystal structure of $WO_3$, ZnO and $WO_3$/ZnO nanocomposite. The $WO_3$/ZnO nanocomposite particles size is 20 nm compare with ZnO and $WO_3$.

# Fabrication, Mechanical, Optical, and Dielectrical Properties of Paper Filled with $SrAl_2O_4$ : Eu,Dy Oxide and Carbon Nanotubes

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**Abstract ID #NNA-1217**

A growing market of flexible electronics increases attention to materials with low cost and easiness in recycling. The cellulose and its derivatives are considered as suchlike materials due to abundance of their natural sources, well-developed technology of production, biodegradability, etc. The composites those are based on cellulose as matrix are principal component of paper electronics that is a fast-growing branch of modern technology. Depending on the fillers these composites can be electrically conductive, magnetic, thermoelectrical, light-sensitive, etc. It was shown that thin film transistors, solar cells, batteries, sensors, and other devices can be created using cellulose materials [1-3].

This study was aimed on preparation and study of paper embedded with $SrAl_2O_4$:Eu,Dy oxide and carbon nanotubes. The first type of filler is known long-lasting and mechanoluminescent phosphor and the second one modifies an electric conductivity and optical absorption of composites. The engineering of physical (mechanical, dielectrical, and optical) properties of composite samples was performed by changing of fillers content in cellulose. For this purpose, nanocellulose water suspensions from non-wood sources, alkyl ketene dimer, oxide and multiwalled carbon nanotubes were added to the fibrous mass of sulfated coniferous bleached cellulose.

The structure and morphology of the dried composite paper samples were studied by means of X-ray diffraction, Raman and IR spectroscopy, optical and scanning electron microscopies. The mechanical, dielectrical, and optical properties were studied and analyzed from viewpoint of the fillers influence on characteristics of composites.

**ACKNOWLEDGMENTS**

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# Plasmonic Nanoparticles for UV-SERS Probing of Biomolecules

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**Abstract ID #NNA-1218**

Raman spectroscopy is a very powerful yet inefficient technique. It is used for detection of various analytes in environmental or forensic sciences, cancer identification, explosion detection and many others. To enhance Raman signal additional plasmonic materials could be used and in this way Surface Enhanced Raman Spectroscopy (SERS) is obtained. Plasmonic silver or gold nanostructures are the most widely used in this research, however they are most efficient in visible and NIR regions. UV spectral region is less investigated but far more interesting. A vast majority of important biomolecules have electronic transitions in this spectral region providing an additional resonance Raman enhancement by several orders of magnitude [1]. In this way UV Surface Enhanced Resonance Raman Spectroscopy (UV-SERRS) provides ultrasensitive detection of biomolecules with low interference from impurities. In our work UV-SERRS at 325 nm laser excitation is exploited for biomolecules such as adenine. We show a vast selection of materials, including aluminum, copper, cobalt, palladium, indium, and silver, as SERS active materials for studies in UV spectral region. We have prepared several structures of these materials using wet chemistry and laser ablation techniques and the obtained results will be presented. These UV-range plasmonic nanoparticles will lay ground for development of cheap, and disposable Raman sensor that is tunable and highly specific to designated biomarker. The development will also advance the fields of nanotechnology, plasmonics, and metamaterials.

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# Effect of Helium Ion Implantation on 3C-SIC Nanomechanical Resonators

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**Abstract ID #NNA-1242**

Silicon carbide (SiC) is a suitable candidate for nanoelectromechanical systems due to its superior mechanical properties. It is also an interesting material platform to study the coupling of mechanical modes with localized spins associated with irradiation-induced defects. Such a spin-mechanical system can be used for quantum sensing applications [1].

The nanomechanical resonators in 3C-SiC are fabricated by standard semiconductor processing techniques and are characterized for resonant frequencies and quality factors. We focus on the material modification by helium ion broad beam implantation on prestressed 3C-SiC resonators. The effect of varying fluence on change in mechanical response is studied. With the fluence $\Phi=1*10^{14}$ ions/cm$^2$, we observe a decrease in resonant frequencies and quality factors. However, we report no change in mechanical properties at lower fluences within the range where hybrid spin-mechanical systems can be realized.

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# Device Engineering and Nanofabrication of Junctionless, Silicon Nanowire-based Wrapped-around Gate Transistors

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**Abstract ID #NNA-1282**

Nanowire (NW) transistors can be seen as the ultimate integration of innovative nanodevices [1], and they are one of the candidates that have sparked significant attention from both device and circuit developers due to their potential for constructing highly dense and high-performance electronic circuits. For achieving high device performance, superior gate control, and better carrier transportation characteristics, excellent control in device architecture of Si NW field-effect transistors (FETs) with wrapped-around gates is being explored nowadays as a possibility for its deliberate use in future CMOS technologies [2].

Herein, a junctionless-NW FET with a wrapped-around gate has been demonstrated from a top-down fabricated Si NW scaled down to 10 nm. An investigation has been conducted on the fabricated devices to analyze and optimize their various physical device performances by systematic device engineering. The gate length ranging from 100 to 500 nm, along with a Si NW channel width variation of 10 to 50 nm, was investigated. Discussions are made also on the optimization of physical parameters, such as the doping value at the channel region, channel length as well as width, and the bias requirement for switching the transistor from the OFF to ON state. We have achieved an ON-current of 10.2 μA for a higher bias setting (VDS=1.5 V) and 0.17 μA for a low bias setting (VDS=50 mV) at a constant value of VGS=2 V for a 10 nm thick and 250 nm long NW-FET. On- to off-current ratios of $1x10^4$ and $2.3x10^4$ were found from a 250 nm and 500 nm long NW FET, respectively. Corresponding subthreshold slopes were found to be 150 and 80 mV/decade, while the associated threshold voltages were -592 and 172 mV. A comprehensive discussion on the entire fabrication process of the nanowire indicates that employing precise patterning techniques can yield improved outcomes. Furthermore, theoretical simulations are performed to validate the experimental results.

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# Laser-Induced Graphene (LIG) Based Electrodes for Biosensing Applications

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**Abstract ID #NNA-1315**

Graphene is one of the most popular 2D nanomaterials with unique physicochemical and mechanical properties. While traditional strategies for graphene synthesis are time consuming and expensive, laser-induced graphene (LIG) can be synthesized using a cheap and rapidly manufactured methodology. Interestingly, LIG allows for the simultaneous production and patterning of nanomaterials without the need for toxic solvents typically used in ink making [1]. It is possible to make LIGs with diverse geometries on various substrates from synthetic polymers to natural biopolymers which is in line with sustainability criteria. LIGs have been successfully utilized as porous electrodes for different applications such as energy storage and (bio)sensing. Chemical functionalities, imperfections, and potential dopants in LIGs' structure, can not only induce favorable properties but also, they can be utilized for surface engineering and immobilization of various recognition elements. However, operating conditions during lasing process significantly affect the properties of the produced LIGs indicating the importance of finely tuning laser parameters. Conductive and porous structure of LIGs enable electrodeposition of various materials from polymers to metal (oxides) nanoparticles. The obtained surface-engineered LIGs can serves as sensing platforms to detect pH range or various analytes such as glucose. Furthermore, coating LIGs with hydrogel membranes (HMs) which can accommodate various bioreceptors or respond to external stimuli is a relatively facile strategy for biosensor manufacturing. In addition, LIGs can be transferred to HMs under vacuum or cryogenic conditions. Integration of LIGs with HMs make diverse platform to make flexible and potentially wearable biosensors. Because of chemical diversity of hydrophilic polymers, it is possible to develop various types of HMs with customized properties such as self-healing, stretchability, electrical/ionic conductivity, antifouling and antibacterial activity, and so forth.

This paper is focused on the applications of LIGs for development of biosensors. Although, bare LIG can be utilized as sensing element, but it is usually modified with biorecognition elements (e.g., enzymes) in order to enhance the selectivity and sensitivity of the obtained biosensor [2]. However, such modifications are not always straightforward and require utilization of appropriate chemistries like bioorthogonal reactions. Here, the importance of LIG coating with polymer, metal (oxide) nanoparticles, and integration of LIGs with HMs, toward biosensing and bioelectronic applications will be highlighted with some of our recent results on LIG-based biosensors. High surface area and high electrical conductivity of LIGs, and hydrated nature of HMs, that mimic natural living tissues, enable favorable signal transduction and stable immobilization of bioreceptors.

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# The Impact of Stoichiometry on the Endurance of Tantalum Oxide-Based Memristors

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**Abstract ID #NNA-1323**

Memristors based on tantalum oxide show great promise for the next era of memory devices, providing strong endurance and retention capabilities crucial for advanced computing and neuromorphic applications. The present work focuses on the significant impact of stoichiometry, specifically the level of oxygen vacancies, on the endurance of these memristors. By conducting a thorough combination of experimental analyses and computational simulations, we explore the complex connection between stoichiometric variations, electrical switching behavior, and the long-term durability of tantalum oxide-based memristive devices.

Our research uncovers a strong link between stoichiometry and the resilience of memristors, highlighting the essential role of oxygen vacancy concentration in shaping their endurance properties. Our results indicate a strong correlation oxygen vacancy concentration on improving memristor performance, vis-à-vis, J-V Characteristics, High Resistive Level (HRL) / Low Resistive Level (LRL) and the corresponding Hysteresis.

Comprehending the intricate relationship between stoichiometry and endurance in tantalum oxide-based memristors is crucial for enhancing their reliability and effectiveness in cutting-edge memory technologies. This study sets the stage for optimizing material composition, thereby driving the advancement of more resilient and long-lasting memristive devices essential for the future of computing and cognitive systems.

## ACKNOWLEDGMENTS

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# Nickel-Zinc Based Nanomaterials for Electromagnetic Communication

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**Abstract ID #NNA-1356**

In recent times the nanomaterials has been a great attention for their exceptional electromagnetic and dielectric applications.The size and shape dependent tunable electromagnetic (EM) properties of NZ nanocomposites makes them an attractive material for various future electronics device applications such as wearable and RF antennas. In this study NiO nanoparticles, ZnO nanoparticles and NZ nanocomposites samples have been synthesized by wet chemical method and electromagetic properties such as, complex permeability, complex permittivity, magnetic and dielectric loss tangents and temperature dependence are studied. X-ray powder diffractometer (XRD) has been used to establish the phase purity and crystal structure. The surface morphology of the samples has been obtained using a scanning electron microscope (SEM). The XRD studies which confirmed the presence of crystal structure of NiO, ZnO and NZn nanocomposite. The NZn nanocomposite particles size is 25 nm compared with ZnO and NiO nanoparticles.

# From Physics to Application: The Development of Quantum Sensor Based on Diamonds with NV Centre Impurities

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**Abstract ID #NNA-1367**

Nitrogen Vacancy (NV) diamond-based sensor enables unprecedented measurement precision and has been demonstrated to be a transformative sensing tool for exploring electrical, magnetic, and thermal features. The technology has already found numerous applications in research, e.g., nanoscale imaging of non-collinear spin textures, optical detection of resonant spin wave modes, non-invasive measurement ferromagnetic materials, analysis of 2D magnetic materials, millimetre-scale mapping of charge current distributions and many others. [1-3] Nonetheless, the consumer market penetration is limited due to the high component and equipment costs, poor energy efficiency and overall sensor size. In order to expand the magnetic field range of NV-based quantum sensing techniques, microwave engineering is required to develop high-frequency, low-loss microwave circuits for NV operation [2]. Some ambitious work [4-5] has managed to integrate microwave excitation structures, optical filters, photodiodes and even microwave generation circuitry directly on a 65nm CMOS chip. The current integrated approaches lack sensitivity, nonetheless, the long-term decrease in costs may enable ever-growing application space. Europe has set a goal to become the world's "Quantum Valley" [6]. Adhering to the call, the Institute of Electronics and Computer Science (EDI) together with partners across Europe implements multiple consecutive EU projects advancing the field of quantum sensing. EDI leverages its unique prior experience collaborating with physicists to improve the applicability of the novel sensing technology. This talk will cover:

- principles of NV diamond-based magnetometry and sensing techniques;
- principal, technical and practical challenges faced during sensor implementation and cross-field collaboration;
- the current stage of the developed technology and its limitations;
- different technology use cases, GNSS-denied localization, predictive maintenance;
- future outlook and key challenges for reaching consumer-grade adoption of the technology.

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TRACK 11

# “NANOMATERIALS FOR ENERGY & ENVIRONMENT”

# Design and Development of Perovskite Solar Cell for Efficient Near Infrared Spectrum Harnessing

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**Abstract ID #NEE-0914**

Conventional lead-based perovskite solar cells typically begin photogeneration at wavelengths around 800 nm, resulting in a significant loss of spectral energy in the near-infrared (NIR) region. Enhancing light absorption beyond 800 nm into the NIR could potentially boost photocurrent generation, thereby enhancing the overall efficiency of perovskite solar cells (PSCs). This study presents a straightforward method to integrate a NIR-absorbing doped metal oxide into perovskite absorbers. This approach aims to broaden the photoresponse range of PSCs and improve their efficiency. The modified solar cells exhibit photocurrent generation in the NIR region, extending beyond the band edge of the perovskite active layer alone. As a result of these improvements, perovskite solar cells featuring the metal oxide additive achieve an enhanced efficiency of 13.9% from 9.92% and notably increased operational stability under continuous one-sun illumination. These findings underscore the potential applicability of directly introducing a multifunctional organic semiconductor into perovskite active layers. This strategy not only extends light absorption towars 2500 nm, but also addresses surface trap issues, leading to the development of highly efficient and stable PSCs capable of harvesting NIR light effectively.

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# Effect of $Sm^{3+}$ on the Structural Properties and Photocatalytic Performance of $TiO_2$&Au Nanocomposites

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**Abstract ID #NEE-0920**

The synthesis of $TiO_2$&Au/Sm particles with gold content of 2 and 4 wt.% and samarium 0.2 wt.% was carried out by the chemical precipitation of a TTIP solution in the presence of $Sm^{3+}$ and $Au^{3+}$ cations. The CSR of nanopowders was 18-20 nm. Aurum is included in the composite structure, which led to an increase in the parameters of the anatase crystal lattice. The presence of samarium in the composite structure was confirmed by EDS and PL methods. The obtained structures showed high sorption activity to cationic dyes (Methylene Blue and Rhodamine B), and lower – to anionic ones, in particular, Orange G. Under the influence of UV irradiation the dye's solutions undergo discoloration, which is accompanied by the destruction of organic molecules, which is confirmed by the hypsochromic shift of the characteristic maximum in the UV-VL spectra. The series OG (46.7 %) < MO (89.2%) < MB (96.0%) < RhB (98.5%) for TiO2&Au/Sm particles ([Au] = 2 wt.%, [Sm] = 0.2 wt.%) and MO (22.6 %) < RhB (24.1 %) < OG (41.5 %)< MB (98.6 %) for TiO2&Au/Sm ([Au] = 4 wt.%, [Sm] = 0.2 wt.%) particles were found according to the intensity of discoloration of the dye's solutions. The difference in the course of the photocatalytic process can be related to the PZC (point of zero charge) of the composite particles, which is 7.01 ([Au] = 2 wt.%) and 9.25 ([Au] = 2 wt.%).

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# Dopant Induced Weak Ferromagnetism in Substituted ZnS QDs And Its Photocatalytic Application

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**Abstract ID #NEE-0927**

Global challenges, such as increasing human energy consumption and resulting environmental damage, are pressing concerns. Photocatalysis, a process that employs light and a catalyst to speed up chemical reactions, holds great potential for eliminating harmful pollutants. The degradation refers to the gradual deterioration of a material over time, often due to chemical reactions or physical wear. Scientists study degradation to gain insights into how materials can be safeguarded or enhanced to extend their lifespan and enhance their performance. The investigation of induced magnetic properties in transition metal-doped quantum dots (QDs) is crucial for applications in spintronic devices. To delve deeper into this, an extensive study was conducted on Co-doped ZnS QDs with varying Co concentrations (x = 0.00, 0.03, 0.06, 0.09) using a combination of experimental and theoretical methods. X-ray diffraction analysis confirmed the presence of pure crystal phases, while high-resolution transmission electron microscopy (HRTEM) images and shifts in absorption spectra validated the characteristics of quantum dots. The weak ferromagnetic behavior observed in the doped samples was attributed to p-d hybridization between Co ions and the valence band of ZnS QDs. Density functional theory (DFT) calculations and finite-difference time-domain (FDTD) simulations provided insights into the blue shifts observed in absorption spectra. Moreover, the dielectric properties were found to be influenced by grain boundaries, with higher Co dopants exhibiting increased polarization loss at low frequencies. The photocatalytic activity demonstrated higher degradation rates in the ZnS QDs with higher Co dopant concentrations.

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# Electrochemical Performance of Hybrid Spinel Ferrite /Carbon ($NiFe_2O_4$/C) Nanocomposite Derived From Metal-Organic-Frameworks (MOF) as Electrode Material for Supercapacitor Application

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**Abstract ID #NEE-0931**

Electric devices and hybrid electric vehicles have raised the demand for large electric energy storage which can be fulfilled by the supercapacitor (SC). Supercapacitors possess superior properties of fast charging, high power density, and long cycle life, so are seeking eminence attention in various fields like photographic flashes, electric vehicles, power emergency actuators in airlines, wearable and foldable electronics, etc. [1–2]. In Electric Double Layer Capacitors (EDLC), carbonaceous materials employ surface adsorption to store charges whereas, in Pseudocapacitors, metal oxides and polymers use redox reactions for charge storage. Due to the usage of redox reaction phenomena for charge storage in Pseudocapacitors, the electrodes must be capable of high electrochemical activities. In this regard, Metal oxides, hydroxides, phosphides, sulphides, and Metal-organic frameworks are being used as electrode materials these days [3-5].

MOFs derived spinel ferrites which are a type of mixed metal oxides are of great interest in energy storage applications due to smaller charge activation energy and enhanced electrical conductivity as compared to other metal oxides derived from MOF [6]. Among various spinel ferrites, Ni Ferrite has been explored much due to its better electrochemical and thermal stability, enhanced redox reaction from various oxidation states, and low cost. Additionally, $NiFe_2O_4$ is non-toxic and, the precursor required for the synthesis is inexpensive and easily available [7-8]. However, agglomeration of NiFe2O4 nanoparticles during synthesis is a major drawback for energy storage applications [9]. It is important to note that, $NiFe_2O_4$ must be obtained in a consistent morphology for charge storage applications.

In present research, Ferrite/carbon ($NiFe_2O_4$/C) nanocomposite derived from surfactant-free Metal-organic frameworks (MOF) has been evaluated as electrode material for supercapacitors. The ferrite/carbon hybrid is synthesized via one step solvothermal method followed by pyrolysis for 2 hours. The thermal treatment has given rise to porous diamond shaped ferrite/carbon nanocomposite. Pyrolysis of MOF has resulted in homogeneous distribution of ferrite on carbon with lesser agglomeration which moderated the active surface area. The material synthesized at 500°C in N2 environment exhibits electric double layer capacitance (EDLC) and pseudocapacitive charge storage mechanism with the highest specific capacitance of 85.5 F $g^{-1}$ at a current density of 0.25 A $g^{-1}$. The high specific capacitance of synthesized material can be attributed to surface redox reaction from a large active surface area. Asymmetric supercapacitor comprised of NF500 and activated carbon has shown a high energy density of 21.31 Wh $Kg^{-1}$ at a power density of 54.72 W $Kg^{-1}$.

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# Monitoring and Optimizing the Biocatalytic Degradation of Efavirenz With Immobilized Trametes Versicolor Laccase on Ti2ntx Mxene: a Lab-Scale Wastewater Treatment Plant Process

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The practical applications of enzymes as biological catalysts are limited by pH sensitivity and temperature intolerance. One of the solutions is to immobilize the enzymes onto nanomaterials support covalently. However, most nanomaterials require functionalizing the nanoparticle surface before immobilising the enzyme by a bifunctional linker.

Herein, the work presents the immobilization of Trametes versicolor laccase onto Ti2N MXene using a bifunctional linker (glutaraldehyde). The work took advantage of the surface termination (O, OH, and F) of the Ti2N MXene, which results from the etching process. Thus, the laccase is directly linked to the MXene, skipping the nanoparticle functionalization step. The prepared biocatalyst obtained a laccase activity of 256 U/mg at multiple pHs (pH 4.5, 5.5, and 6.5) compared to the free laccase, signifying pH tolerance. The biocatalyst was then used in the combined degradation of ARVs in wastewater by an activated sludge system coupled with a bioreactor and efavirenz serving as a model ARV. The simulated lab-scale treatment plant was operated using the OECD 303A guidelines. A 20.3% and 30.9% efavirenz removal was obtained at sludge retention times 5 and 6 for 5 ppm and 25 ppm, respectively. The combined system showed potency as efavirenz degradation improved to 38.1% and 40.9%. Furthermore, the possible degradation was identified as 6 degradation products using LC-MS.

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# Innovative Development Of Si-Ge Alloy Enhanced with Nanoprecipitates by Additive Manufacturing

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**Abstract ID #NEE-0961**

Thermoelectric (TE) effects encompass reversible phenomena observed in both conductor and semi-conductor materials that allow conversion of thermal energy into electrical energy and vice-versa. TE devices present an environmentallty-friendly technology useful for several niche applications in electricity generation and cooling systems. Traditional manufacturing methods such as hot pressing, zone melting, or spark plasma sintering have enabled the production of cuboid-shaped TE devices. However, the limitations in shapes diversity restrict integration and yield potential of this technology. Consequently, there is a growing focus on leveraging Additive Manufacturing (AM) techniques for TE materials, aiming to overcome these constraints. AM techniques enable also eco-friendly manufacturing compared to standard techniques thanks to a reduction of material losses during manufacturing. Among the various AM methods, Laser Powder Bed Fusion (L-PBF) stands out as a prominent approach for printing complex metal parts in small to medium series. Recent advancements in L-PBF processing have paved the way for the fabrication of novel materials, including TE materials such as bismuth telluride [1-3] and Half-Heusler [4].

Our work presents the development of silicon germanium alloys TE material, tailored for applications at high temperatures. It is the first time that this material has been manufactured by L-PBF process. The first developments for the manufacturing of this material resulted in a dense material with promising Seebeck coefficient and thermal conductivity, but with mechanical cracking occuring during L-PBF processing due to material induced stresses. To address this issue, a new approach was studied : nanoprecipitates formation during cooling based on powder mixing of raw SiGe powder and nanoparticles. Nanoprecipitates can simultaneously enhance TE properties by scattering phonons and enhance mechanical properties, by acting as nucleating agents for silicon germanium matrix and thus reduce grain size. It is the first time that such approach is applied in AM of TE materials.

A specific study has been performed to define the best nanoprecipitates candidates. Three systems of nanoprecipitates were retained, based on SiC, WSi2 and MoSi2. This work will present how these nanoprecipitates have been chosen, then their impacts on SiGe structural properties. The influence of precipitates size, interfaces, and matrix microstructure will be also presented. Finally, the impact of nanoprecipitates on SiGe TE properties will be discussed.

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# Engineered $Ti_3C_2T_x$ MXene Based Multifunctional Electrocatalyst for Wastewater to Hydrogen Generation and Treatment

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**Abstract ID #NEE-0971**

Hydrogen generation via wastewater (WW) splitting is a sustainable approach to producing green hydrogen fuel. Over the last few years, enormous efforts have been made to develop an efficient electrocatalyst for exploring low-grade water or WW utilizing various oxides. Lately, MXenes i.e., transition metal carbides, nitrides, and carbonitrides, have gained significant attention as an electrocatalyst due to their superior electrical conductivity and active basal planes. However, they are not fully studied in a WW environment as a multifunctional catalyst, which offers more challenge due to presence of contaminants.

In the present work, a commonly used MXene i.e., $Ti_3C_2T_x$ is engineered by decorating it with transition metal alloys i.e., NiCo and NiMo via optimized electrodeposition. The synthesized catalysts are characterized for their structural, optical, elemental compositions, morphological properties, etc., to confirm their synthesis. The polarization studies revealed that NiMo/$Ti_3C_2$ and $Ti_3C_2$/NiCo exhibited an overpotentials of 45.8mV and 36.6mV, respectively, at 10mA/cm2 in alkaline WW, generating approximately 0.361 to 0.603mmolh-1 of hydrogen from industrial wastewater. Additionally, NiMo/$Ti_3C_2$ and $Ti_3C_2$/NiCo achieved excellent methylene blue (MB) degradation of ~82% and 86%, respectively. A scavenger study reveals the role of reactive oxygen species (ROS) in pollutants degradation, while electrons for hydrogen generation. The promising catalytic activity of the engineered $Ti_3C_2$ could further be assigned to synergistic contributions from MXene and transition metals. In addition, this study also contributes to the multifunctional activity of MXene for simultaneous wastewater treatment and hydrogen generation.

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# Plasma Synthesis of Multifunctional Thin Films and 3D Nanoarchitectures for Energy Harvesting Applications

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**Abstract ID #NEE-0982**

Single- and multi-source environmental energy harvesters and nanogenerators will promptly pave the way for the realization of Industry 4.0 and Smart Cities. However, advances are yet required in the design of functional nanomaterials, and their synthesis and processing procedures.

In this presentation, we will demonstrate the application of vacuum and plasma-assisted deposition techniques to process surfaces and thin films and to develop complex nanowires (NWs) and nanotubes (NTs) with a core@multishell morphology where each shell adds functionality or multifunctionality to the system. The steps required for the implementation of these nanomaterials as supported or in-device applications will be presented together with our latest accomplishments in the field of solar cells, [1-4] piezoelectric and triboelectric nanogenerators [5-7] and self-powered sensors.

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# Synthesis of High-Quality Expanded Graphite from Flotation-Enriched Natural Graphite

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**Abstract ID #NEE-0987**

It is known that more than 50 % of power equipment shutdowns, which cause large losses, occur due to a violation of its tightness. The most reliable and widely used in the world are seals made of expanded graphite (EG). Natural graphite with a carbon content of > 99.0 % wt. is used as a raw material for the production of EG seals for thermal energy, petrochemical, etc. equipment, and 99.9 % wt. for nuclear power plant equipment, which are quite expensive. The synthesis of EG is a multi-stage process that includes its oxidation with sulfuric acid with the participation of strong oxidants ($KMnO_4$, $K_2Cr_2O_7$) or nitrate acid, hydrolysis, washing to neutral pH, drying, heat treatment, and mechanical rolling and pressing. Such processes create a large environmental load.

In this work we show that the combination of oxidized graphite synthesis process (graphite intercalation by anodic treatment in concentrated sulfuric acid, followed by hydrolysis) and chemical purification using solutions of ammonium bifluoride in sulfuric or hydrochloric acid and trilon B in alkaline buffer, as cleaning reagents, allows you to obtain high-purity EG with a carbon content of more than 99.5% wt. from flotation-enriched graphite with a carbon content of 94-97% wt. The optimal process parameters are given in [1]. The methods of X-ray phase analysis and thermogravimetry show that the interaction of oxidized graphite with cleaning reagents does not reduce the ability to expand. The magnitude of the mass loss of oxidized graphite according to various variants of chemical post-cleaning and the temperature range of such loss remain practically unchanged. The main mineral impurities in graphite ore are aluminosilicates up to 60-80% wt., which effectively interact with the hydrofluoric acid that is formed, and oxides of iron, calcium and magnesium. Quantum chemical calculations show that the trilon B molecule is better physically sorbed on the oxidized graphene-like plane (– 412 kJ/mol) than on its native form (– 188 kJ/mol). The interaction of trilon B with $Ca^{2+}$ and $Mg^{2+}$ cations, regardless of the nature of the cation, is thermodynamically more likely in an aqueous solution than in the adsorbed state on the surface of the oxidized graphene plane. The proposed method provides high-purity EG, significantly reducing the cost of the technology and reducing environmental pollution.

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# 2D Perovskite Thin Films with Controlled Properties for Opto-Electronic Applications

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**Abstract ID #NEE-0992**

Metal halide perovskites (PVK) have emerged as one of the most promising family of semiconductor materials for applications in various fields such as lasers, light emitting diodes, photodetectors, scintillation and photovoltaic solar cells.[1,2] For their commercialization, their present rather low stability remains a serious issue. The stability and property tuning of metal halide perovskite films can be enhanced by employing halide perovskites with lower dimensionality as an overlayer, or at the grain boundaries. 2D halide perovskites, with crystal structure stabilized by monoammonium (A') organic cation spacers, can also be directly employed as the active layer. Ruddlesden-Popper (RP) phases, with molecular formula A'2An−1BnX3n+1 (with A being a monovalent cation, B being Pb2+ or Sn2+ and X being a halogen), are known to be more stable than their 3D counterpart.

In the present talk, we will develop various important aspects related to the integration of 2D Perovskites in optoelectronic devices. We will describe and discuss the formation process of the layer with a special focus on the annealing effect. We will then present results on the use of the 2D RP perovskites in solar cells.[3] We will subsequently develop the employment of 2D RP (n=2) perovskites, for two different A' spacer cations, in flexible photodetectors [4,5]. We will finally show how integrated flexible PDs arrays have been used as effective visible light image sensors with good spatial resolution.

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# The Influence of Magnesium Doping on the Structural Characteristics of $Cu_2ZnSnS_4$ Nanoparticles Obtained by the Polyol Method

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**Abstract ID #NEE-1007**

Four-component kesterite compounds like $Cu_2ZnSnS_4$ (CZTS) and $Cu_2ZnSnS_4$ (CZTSe) are promising for thin-film solar cell absorber layers and thermoelectric elements. This dual functionality allows for the creation of hybrid devices that incorporate solar cells and thermoelectric elements using a single material. Classical kesterite compounds like CZTS have a notable limitation in thermal devices due to their low electrical conductivity. Introducing magnesium into the material shows promise for enhancing electrical conductivity by providing additional charge carriers. We demonstrate the synthesis of this compound using the polyol method, which offers advantages such as simplicity, scalability, and cost-effectiveness. It is known that substituting $Mg^{2+}$ ions for $Zn^{2+}$ ions in the crystal lattice of the compound slightly increases the lattice parameters of the CZMTS solid solution due to the larger covalent radius of $Mg^{2+}$ (0.136 nm) compared to $Zn^{2+}$ (0.125 nm). The analysis of transmission spectra indicates a decrease in the bandgap width of the compound from 1.49 eV to 1.07 eV (CMg = 40%) with an increase in Mg concentration, which then rises to 1.27 eV (CMg = 60%). We expect that our synthesized magnesium-doped nanoparticles of $Cu_2Mg_xZn_{1-x}SnS_4$ (CZMTS) solid solutions will be highly effective for thermoelectric applications. To optimize the synthesis conditions, we examined how the magnesium content affects the structural and optical characteristics of the nanoparticles. Substituting $Zn^{2+}$ with $Mg^{2+}$ introduces additional holes into the material, enhancing its electrical conductivity, essential for developing highly efficient thermoelectric devices.

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# Effect of Fullerene Additives on the Optical and Thermodynamic Properties of Eicosane

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**Abstract ID #NEE-1017**

Nowadays, nanomaterials are increasingly used in power equipment as the working fluids, thermal storage materials and heat transfer media. Additives of nanoparticles in the liquid and solid phases significantly change the optical and thermophysical properties of basic materials. However, the mechanism of nanoparticles influence on the optical and thermophysical properties of the basic fluids is still insufficiently examined. The main problems in studying the effect of nanoparticles on the properties of basic materials are the aggregative stability of nanomaterials obtained using different methods as well as lack of comprehensive studies of different optical and thermophysical properties for identical samples of the nanomaterials. In order to solve this question a comprehensive investigation of the properties for the model thermodynamic system eicosane/fullerene C60 that is a stable molecular solution was performed. New experimental information on the temperature and concentration dependences for the refractive index, light transmission coefficients (at the different wavelengths), viscosity, heat capacity and enthalpy difference at the diffuse phase transition have been obtained. It was shown that changes in the optical and thermophysical properties for the eicosane/ fullerene C60 solutions are determined not only by concentration, size and shape of nanoparticles but also by changes in the structure of eicosane due to presence of the fullerene additives. The structural changes in eicosane related to fullerene additives were investigated by X-ray diffraction experiment and structural analysis.

# Sedimentation Stability and Caloric Properties of Nanohybrid Composite Thermo-Accumulating Material Paraffin/Thermally Expanded Graphite/Copper Oxide Nanoparticles

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**Abstract ID #NEE-1019**

The promising direction to increase the thermal conductivity of composite thermal-accumulated storage nanomaterials (CTNM) is introducing various carbon nanomaterials with high thermal conductivity into paraffin. However, the solution of the problem for the sedimentation stability of the proposed CTNM samples remains poorly examined.

As a solution to increase the sedimentation stability is an application of the thermally expanded graphite (TEG) as a porous nanostructure. However, a small concentration of TEG does not provide the creation of the CTNM with high values of thermal conductivity. In order to increase the thermal conductivity of the CTNM, we propose to fill the matrix of the TEG with nanomaterial paraffin/CuO nanoparticles.

The first stage of the reported method is creation of a deaerated paraffin/CuO nanofluid that was sedimentationly stable for several days. The stability of the created solution was studied by spectrophotometry in the temperature range from 50 to 60 C and wavelengths from 325 to 1000 nm. At the second stage, the TEG at the temperature of 200 C was subjected to deaeration in order to remove air components. At the third stage, the vacuum impregnation of TEG with paraffin/CuO nanofluid was carried out. The technological characteristics were studied: leakage of nanofluid from the porous structure, changes in the composition of the composite material throughout the volume of the sample, etc. At the final stage, new experimental data for the density, thermal conductivity, heat of phase transition have been obtained.

The experiments show that minor additives of the TEG (up to 4%) and CuO nanoparticles (up to 0.6%) contribute to increase in phase change heat (up to 25%) and thermal conductivity (from 0.247 to 2.339 W/(m·K)) compared to technical paraffin. The implementation of the proposed method for producing hybrid CTNM will improve the efficiency of thermal storage devices.

# Nanoparticles as Catalysts in Esterification and Transesterification Reactions

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**Abstract ID #NEE-1027**

Nanoparticles have emerged as promising catalysts for a wide range of chemical transformations, such as esterification and transesterification reactions. These reactions are widely used in the production of biodiesel, pharmaceuticals, food, cosmetics, plasticizers, lubricants, and many other industrially relevant compounds. However, the use of conventional catalytic systems like mineral acids or strong bases in these reactions often encounters issues such as corrosiveness, side reactions, the requirement for catalyst isolation, and their environmental impact. Therefore, the search for new catalysts is still relevant today. In this study, tungsten disulfide (WS2) nanoparticles were investigated as a heterogeneous acid catalyst in esterification of oleic acid, a mixture of oleic and linoleic acids, and transesterification of triglycerides to improve the efficiency of these processes. Nanoparticles have unique properties, such as high surface area, tunable morphology, enhanced catalytic activity, and easy removal from the reaction mixture, which make them promising candidates for catalyzing esterification and transesterification reactions in batch and continuous processes. The primary challenge in developing efficient heterogeneous esterification and transesterification systems is the immiscibility of the oil and alcohol phases, leading to decreased interaction. In this study, ultrasonication was applied to address this issue and improve the mixing of the organic phases and the solid phase catalyst. The use of ultrasonic treatment facilitated the conversion of oleic and linoleic acids to the corresponding ester products with high efficiency and selectivity (yield 95-98%). However, the transesterification process was less efficient. The obtained results will give a background for further investigation of nanoparticles as catalysts in the esterification and transesterification reactions.

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# Biodiesel Production from Brown Grease Using $MoS_2$ and $WS_2$ Nanoparticles as Catalysts: a Sustainable Approach to Alternative Fuel

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**Abstract ID #NEE-1028**

The increasing energy demand, along with the depletion of nonrenewable fossil fuel reserves, highlights the need to explore alternative, eco-friendly energy sources. Biodiesel, made from renewable feedstocks, offers a promising way to reduce environmental pollutants linked to traditional fossil fuels. However, the widespread use of edible oils for biodiesel production raises concerns about global food security.

To tackle this issue, we examine the potential of brown grease (BG), a food industry waste byproduct, as a sustainable source for biodiesel manufacturing. BG, rich in free fatty acids and triglycerides, provides ample raw materials for biodiesel synthesis. Our research delves into the production of biodiesel using BG as a substrate, employing ultrasonic activation and MoS2 and WS2 nanoparticles as heterogeneous catalysts. We introduce an innovative approach for biodiesel production from BG, addressing the challenge posed by its high free fatty acid content. By optimizing the process with ultrasonic activation, biodiesel can be produced from BG within minutes at room temperature. The use of heterogeneous MoS2 and WS2 nanoparticles allows simple separation of the catalyst from the reaction mixture and its repeated or continuous use.

Our findings indicate that the WS2 catalyst exhibits high catalytic efficiency, achieving conversion rates of more than 90%, while MoS2 shows lower performance in catalyzing the reaction. This study not only highlights the potential of BG as a sustainable biodiesel feedstock but also offers a viable and eco-friendly solution to meet the rising energy demands. Our findings pave the way for the creation of efficient, cost-effective, and environmentally friendly strategies for biodiesel production, promising a more sustainable energy future.

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# Long-term Effect of Hydrogen and its Mixtures on Polyethylene Macromolecules

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**Abstract ID #NEE-1037**

Existing ecological trends in replacing of the natural gas as main fuel both for industry and private consumers create new challenges for polymeric science as well as for the science in general. The work presents results of complex investigations of the long-term effect of hydrogen-methane mixtures on the structure and properties of PE80 polyethylene (previously being in operation in gas pipelines for 15 years) for a period of 1 year. Two hydrogen-methane gas mixtures in 10% $H_2$/90% $CH_4$ and 20% $H_2$/80% $CH_4$ proportions have been used for these investigations.

Thermo-gravimetric analysis results showed the formation of a more homogeneous structure, that is, by reducing the number of heterogeneity zones, simultaneously with an increase in their volume. No significant changes in the values of thermophysical parameters of both samples of polyethylene before and after hydrogen mixtures exposure within the range of temperatures of start of destruction $T_{sd}$ and of the maximum of destruction intensity $T_{md}$. In the interval of temperatures of destruction intensity maximum $T_{md}$ and finish of destruction $T_{fd}$ one can observe certain decrease of the temperatures of the processes and increase of their intensity, and this can indicate the destruction of structures with lower thermal stability under the gas mixtures effect.

Differential scanning calorimetry results showed the conjunction of melting peaks of the crystalline phase which indicates its reorganization into more homogeneous, i.e. crystalline phase of polyethylene that had few types of crystals in the parent samples has been changed to the structure of similar crystals. Another characteristic for these samples was decreasing of crystallinity degree $\chi$ after 10% $H_2$/90% $CH_4$ gas mixture effect, and increase after effect of 20% $H_2$/80% $CH_4$ gas mixture. Basing on this we can conclude that separate effect of hydrogen and natural gas can provide competing effect on the crystalline phase of polyethylene, when methane promotes destroying of crystals, and hydrogen promotes its formation.

Based on results of X-ray structural analysis of material, was found crystaline structure changes under the effect of gas mixtures, in particular, new crystal peaks appear at $2\theta$ max $\approx$ 15,9°, and also the intensity of peaks increases at $2\theta$ max $\approx$ 29,5° and 35,5°, which is associated with the growth of polyethylene crystallinity [1]. It was established that the relative degree of crystallinity $\chi$cr of material, that were under the effect of gas mixtures 10% $H_2$/90% $CH_4$ and 20% $H_2$/80% $CH_4$, respectively, is higher in comparison to the parent material.

From the comparative infrared spectra before and after 1 year of polyethylene samples exposure, it can be seen that the chemical structure of polyethylene did not show any changes, resulting from the absence of new or shifts in existing peaks that are responsible for chemical bonds or groups of atoms.

## ACKNOWLEDGMENTS

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# Pyroresistive Properties of Segregated Composites Based on Amorphous and Semi-crystalline Polymers

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**Abstract ID #NEE-1043**

Pyroresistive composites are gaining prevalence across diverse industrial sectors. Pyroresistive effect refers to the generation of Joule heat within an electrically conductive composite upon the passing of an electric current. This makes pyroresistive composites useful for protecting a number of devices, such as electric vehicle batteries, from the harmful effects of cold climates that prevail in northern regions. Low temperatures not only diminish device performance but also pose risks of damage, making the application of pyroresistive composites crucial for ensuring operational efficiency and longevity.

The segregated composites were prepared by the hot-compaction method under a temperature higher than melting point and at a pressure 25 MPa. As an amorphous polymer matrix, polyvinyl chloride (PVC) was chosen with an average particle size of 90-110 mcm. As a semi-crystalline polymer was taken high density polyethylene (HDPE) with particle size in the range 100-150 mcm. The same fillers were added in both matrixes, namely carbon black (CB), chopped carbon fibers (CF), and their mixture.

A comparative analysis between HDPE-based [1] and PVC-based [2] composites, both containing the same carbon fillers amount and having identical sample geometry, reveals comparable values of pyroresistive parameters. The primary distinctions between HDPE and PVC-based composites lie in the conditions required to reach equilibrium temperature. It was demonstrated that equilibrium temperatures are attained at a voltage near the onset of the positive-temperature coefficient (PTC) effect.

Based on the analysis of the experimental data, it is evident that PVC-based composites exhibit higher equilibrium temperatures ($T_{eq}$) at increased voltages ($U_{eq}$) before the emergence of signs of the PTC effect. This phenomenon can be attributed to the semi-crystalline nature of HDPE, which experiences a notably stronger PTC effect compared to amorphous PVC. Consequently, the PTC effect manifests in HDPE composites at lower temperatures and voltages than in PVC composites, resulting in lower Teq and Ueq values in the equilibrium state before reaching the conditions for the PTC effect.

Such materials can be widely used in different types of equipment, various sensors, heating devices, and for plastic welding.

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# Magnesium Substituted Copper Ferrite as an Effective Catalyst for the Organic Dyes Decomposition

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**Abstract ID #NEE-1046**

In this study, a series of magnesium-substituted spinels with general compositions of $Mg_xCu_{1-x}Fe_2O_4$, where x varies from 0.0 to 1.0 a step of 0.2, was synthesized via the sol-gel autocombustion method. Citric acid is used as the chelating agent. The phase composition, particle size, and morphology of the materials were characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), and X-ray dispersion analysis. The effects of magnesium substitution on the magnetic properties of the samples were evaluated using a vibrating sample magnetometer (VSM). Additionally, degradation tests were conducted using a spectrophotometer, with methylene blue (MB) selected as the model pollutant.

The study demonstrates alterations in the structure and magnetic properties of the synthesized material. The spinel produced via self-combustion was found to be a mesoporous material with good magnetic properties. The band gap of this photocatalyst ranges from 1.58 to 2.03 eV, allowing it to be effectively activated by visible light. Degradation tests using methylene blue as a pollutant showed effective dye removal, achieving 95% efficiency within 160 minutes. The copper spinel modified with magnesium ions proved to be an environmentally safe, stable, and effective photo-Fenton catalyst that is simple to synthesize and suitable for practical applications.

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# Single-step Electrochemical Fabrication of Ultrathin Graphitic Carbon Nitride Nanosheets via Platinized Titanium Electrodes for Photo-based Industrial Dye Wastewater Treatment

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**Abstract ID #NEE-1055**

The textile industry poses a global pollution issue due to the inadvertent release or improper disposal of contaminated wastewater into water bodies, significantly impacting the quality of water resources. Approximately 17-20% of industrial water pollution is attributed to textile dyeing and treatment activities, as highlighted by the World Bank's findings. The photo decolorization of dyes has gained attraction as a promising technique for treating industrial wastewater, owing to its environmentally conscious approach, cost-effectiveness, and absence of secondary pollution. Graphitic carbon nitride, often denoted as g-C3N4, stands out as a prominent 2D material in photocatalysis. This metal-free polymeric compound is primarily composed of carbon and nitrogen atoms. The material's electron-rich characteristics have propelled it into the spotlight for researchers intrigued by its properties in photocatalytic and photovoltaic processes. Consequently, g-C3N4 has gained substantial attention as a preferred photocatalyst in various redox reactions. In this work, we opted for an electrochemical method for the synthesis of g-C3N4, an environment-friendly approach. Its structural, chemical, morphological, and optical properties were characterised by using X-ray diffraction (XRD), transmission electron microscopy (TEM), Scanning Electron Microscopy (SEM), Fourier-transform infrared spectroscopy (FTIR), UV/Vis spectroscopy, and photoluminescence spectroscopy. We performed a group of experiments using a set of dyes (cationic and anionic dyes), and we found that the catalyst showed up to 98% photo-assisted decolourization of dyes in an alkaline medium.

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# Cyanobacteria Immobilized Rgo-Ppy/Ito-Pet Nanocomposite Based Photo-Bioanode for Bio Electricity Generation towards Non-Mediated Bio Photovoltaic Cell Application

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**Abstract ID #NEE-1058**

The current global environmental and energy issues have spurred a quest for an alternate, sustainable energy source to address the increasing worldwide energy demand. Bio-photovoltaic cell (BPV) technology has garnered significant attention from scientists as it presents an opportunity to merge biological processes with photovoltaic technology in order to convert light into electrical energy. The advancement of bio-photovoltaic cells is heavily reliant on the development of electrode materials that can efficiently catalyze the essential electrochemical reactions in these devices. Thus, there is a crucial requirement to explore suitable electrode materials that exhibit outstanding conductivity, high specific surface area, biocompatibility, and chemical stability in order to improve bio-photovoltaic device performance.

Utilizing new or modified 2D electrode nanomaterials with inherent conductive properties could enable the creation of high-performing bio-photovoltaic cells capable of generating substantial power output. Employing graphene and its nanocomposites with conductive polymers in BPV demonstrates promising outcomes compared to traditional ITO and carbon-based electrodes due to their enhanced conductivity and large surface area which facilitates effective adsorption of cyanobacteria leading to increased power production and durability. This research focuses on producing an efficient rGO-PPy nanocomposite-based anode for electricity generation using cyanobacteria as a biocatalyst in photoelectrochemical cells. Immobilizing Nostoc sp. on the fabricatedelectrode displays strong electrocatalytic activity resulting in enhanced power generation within electrochemical fuel cell setups, paving the way for cost-effective construction of highly efficient BPVs.

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# Structure and Electrical Properties of Polyaniline/MAX Composites

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**Abstract ID #NEE-1079**

MAX phases are a large family of materials extensively investigated in recent years due to layered structure and a unique combination of metallic and ceramic properties, such as high thermal and electrical conductivity, mechanical strength, low density, resistance to high temperatures and oxidation. [1, 2]. Thus, MAX phases are suggested to have potential applications as a high-temperature structural material, protective coatings for refractory alloys, bond-coat layers in thermal barrier coating systems on aero-engines and other gas turbines, accident-tolerant fuel cladding in nuclear power plants, heat exchangers, solar receiver in concentrated solar power systems, electrical contacts, catalysts [2]. Moreover, the interest in MAX phases has increased significantly in recent years as they are the precursors for MXenes. A large number of publications on these materials and their applications appear annually. It has been reported that MAX phase/conducting polymer nanocomposite can be used as an excellent photocatalyst [3] and for supercapacitor electrodes with improved thermal and mechanical properties [4]. However, the effect of the MAX phase introduction on the properties of conducting polymers has not been sufficiently studied. In this work, we investigated the influence of MAX phase, namely Ti2AlC, on the structure and electrical properties of polyaniline (PAn).

The samples of PAn/MAX composites powder were obtained by "in situ" oxidative polymerization of aniline using an equimolar amount of ammonium persulfate as oxidant in a medium of 0.5 M toluene sulfonic acid in the presence of 0,05–30 wt% Ti2AlC. The IR spectra analysis of PAn/MAX composites indicates the possible interaction of the polymer's functional groups with the inorganic filler. Characteristic IR oscillations of PAn-TSA are observed in all samples. According to the X-ray diffraction analysis, the effect of the filler on the composite structure becomes visible when the MAX content is within 3–5 wt. %. The SEM images of the surface of the composites were analyzed, and the electron density distribution map was obtained. Due to the elemental analysis results, increased MAX concentration in the reaction solution leads to higher titanium and aluminum content in composites. The SEM images of PAn/MAX reveal mostly the amorphous uniform structure with individual MAX granules distributed over the entire surface area. Based on the temperature dependence of the specific resistance of the composites in the range of 293–373 K, the activation energy of conductivity Ea and its dependence on the filler content were determined. It has been observed that the value of Ea decreases with an increase in the MAX content in the polymer composite.

## ACKNOWLEDGMENTS

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# Expeditious Arsenic Removal from Drinking Water by An Iron-Manganese Binary Oxide Nanoparticle-Nylon 6 Fibre-Based Adsorbent

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**Abstract ID #NEE-1086**

Arsenic in drinking water causes serious health problems [1] and must be brought below the permissible 10 ppb limit [2] rapidly, for on-spot remediation. Household reverse osmosis (RO) units are unable to remove As(III) completely, which is more poisonous compared to As(V) [3]. It removes 99% of As(V) and around 60–70% of As(III) from the water [4,5]. To address this, a post-RO adsorbent is developed based on iron-manganese binary oxide nanoparticle impregnated nylon 6 fibre (IMBNP-nylon 6) to remove 30 - 40 % As(III) that remains in the permeate water following the membrane separation step in the RO process. In this work, we restricted the growth as well as the aggregation of impregnated binary oxide nanoparticles on the polymeric fibre by employing a combined new approach of acid treatment and reduced temperature impregnation and vacuum drying. The outcome of these efforts was an increase in the loading amount of particles on fibre from 1.4 to 9.3–10 wt%, giving a high adsorption capacity of 48.7 mg As(III)/g of IMBNP-nylon 6 fibre. This system, on using a very small 3.9 cc glass column with either 100 or 38 ppb As(III) feed solution [with a very short contact time (39 seconds)], could treat and purify as much as 5,200 or 21,000 times bed volume of arsenic contaminated drinking water, respectively.

The key advantage of IMBNP-nylon-6 fibre is that it provides low resistance to liquid flow through it, which avoids the channeling of water streams. This facilitates its higher efficiency for As(III) removal than that of a powdered or granulated bed. Additionally, this experiment revealed that the concentrations of iron and manganese leached into permeate water are less (10 ppb for iron and 50 ppb for manganese) than the permitted amount, which is 300 ppb for iron and 50 ppb for manganese, respectively. Overall, this work demonstrates the potential scalability of this technique to treat a large amount of arsenic-containing permeate water in household RO units.

## ACKNOWLEDGMENTS

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# Novel Amine-Functionalized Silica Xerogels for the Adsorptive Removal of Quinolone, β-lactam and Macrolide Group Antibiotics from Water

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**Abstract ID #NEE-1090**

Amine functional silica-based aerogel/xerogels are one of the most attractive materials in separation applications due to their porous network and high affinity for various contaminants such as $CO_2$ and heavy metals. Recently, these structures have also been found to be efficient in capturing high-concern antibiotics from wastewater [1,2]. In this study, it was aimed to synthesize a novel amine-modified organic-inorganic silica hybrid adsorbent for the removal of various antibiotics from the aqueous media. For this, a new amine functional silane (bis[3-(triethoxysilyl)propyl]amine-BTESPA having a long organic chain containing six functional amine groups was selected as a silica source. The adsorbents were prepared by the one-step sol-gel method under ambient conditions without using any catalysts. Benefiting from the self-catalyzing property of the selected amino silane, complete gelation occurred only within 1 h. The chemical and structural characteristics of the xerogels were revealed by FTIR, SEM, SAXS, and $N_2$ sorption analyses. Antibiotic adsorption performances were evaluated via batch-sorption experiments by selecting different quinolone, β-lactam, and macrolide group antibiotics, respectively.

Characterization results have indicated typical mesoporous structures for xerogels with high apparent surface area (> 500 $m^2/g$) and low density (< 0.2 $g/cm^3$) values. Thanks to the well-developed porous network and the silica surface decorated with nucleophilic amine groups that may facilitate the sorption of organic molecules, the synthesized xerogels have displayed highly promising sorption results with repeatable cyclic performances (up to 6 cycles). At the optimum operating conditions, maximum sorption capacities were found to be 64.5 mg/g, 57.2 mg/g, and 103.8 mg/g for quinolone, β-lactam, and macrolide group antibiotics, respectively. The combination of time-saving and facile synthesis strategy together with the high sorption capacity makes these new amine-functional silica xerogels emerge as promising adsorbents for the removal of pharmaceutical compounds from water..

## ACKNOWLEDGMENTS

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# Effect of Concentrated Solar Radiation on the Surface Structure of Cathode of a Low-Temperature F-TEC Based on the TiH–TEG Composite

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**Abstract ID #NEE-1097**

The production of energy by traditional methods using fossil fuels contributes to the deterioration of the ecological situation. One of the most common alternative energy sources is solar cells, which require large areas for solar farms, create environmental problems in their production and utilization, and have a low specific power. More efficient and environmentally friendly are direct thermionic energy converters (TECs), whose use is currently limited by their high operating temperatures. Therefore, the search, synthesis, and investigation of materials that would ensure a decrease in the operating temperature of TECs is an important and urgent task. Preliminary studies on the electrophysical properties of the virgin hydrogenated titanium–thermoexpanded graphite (TiH–TEG) powders have shown the formation of a nanocomposite, and also that a photo-thermionic energy converter (F-TEC) with a cathode made of a composite TiH + 0.53 wt% TEG and with caesium atoms in the vacuum interelectrode space, in a solar concentrator at temperatures of 170-350°C, exhibits voltage and constant current in a closed electric circuit without applying any additional external potential difference. In this paper, SEM and AFM methods were used to study the change in the surface morphology of cathodes based on the composite TiH + 0.53 wt. % TEG under the influence of concentrated solar radiation and corresponding temperatures. During rapid (significantly non-equilibrium) heating in the solar concentrator, new carbon nanostructures are formed on the metal particles of the composite samples. These structures form a thin layer of amorphous carbon with sp3-hybridized bonds, which is evidenced by a threefold increase in the ratio of the intensities of the D and G peaks (ID/IG) on the Raman spectra before and after solar irradiation. The significant restructuring of the surface is also confirmed by X-ray diffraction data, while no similar surface restructuring is observed during slow annealing in a vacuum furnace. After solar irradiation, the surface roughness of the cathode increases significantly: the formed carbon nanostructures have the form of separately located icicle-like growths with diameters of 20–500 nm and a height of up to 140 nm which can provide an increase in the contribution of field electron emission during further operation of the cathode. The appearance of a large number of new carbon nanostructures on the surface of hydrogenated Ti particles and the diffusion of hydrogen from the volume of metal particles to their modified surface increase the emission efficiency of the F-TEC cathode by increasing the working area of its surface and using various mechanisms of electron emission, including generation under the influence of light "hot" electron population.

**ACKNOWLEDGMENTS**

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# Fabrication of Nanocomposite Adsorbent Based on Manganese Dioxide-loaded Zeolite for Enhanced Removal of Cadmium from Contaminated Waters and Soils

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**Abstract ID #NEE-1117**

Over the last few decades, the contamination of natural waters and soils with heavy metals has become a serious problem in terms of human health and impact on the environment. Cadmium is one of the most toxic elements to humans. Environmental releases of Cd from anthropogenic activities such as mining, smelting, production of pigments and cadmium-nickel batteries, and the use of phosphate fertilizers have severely affected water and soil quality and increased the risk of human exposure. Among the methods used to remove cadmium from sewage and contaminated soil (such as chemical precipitation, membrane filtration, adsorption, ion exchange and electrodialysis), adsorption has proved to be the most effective and economical due to its simplicity, ease of operation and low cost.

Hydrated manganese dioxide with a layered structure (birnessite) is well known as an efficient material for the selective removal of Cd ions through inner sphere complexation. However, birnessite is usually synthesized in the form of ultra-fine particles. The low hydromechanical stability of as-synthesized birnessite and its tendency to agglomerate limit its practical application. The synthesis of composite materials with manganese dioxide nanoparticles has made it possible to overcome the above-mentioned drawbacks.

The paper presents the results of the synthesis of a composite adsorbent for the selective removal of Cd ions based on clinoptilolite tuff from the Sokyrnytsia deposit (Ukraine) loaded with manganese dioxide nanoparticles. The successful synthesis of the nanocomposite adsorbent was confirmed by X-ray diffraction, Fourier transform infrared spectroscopy, Scanning electron microscopy and Zeta potential techniques. Samples of natural and composite clinoptilolite tuff were tested for selective removal of Cd ions from model solutions with high content of competing ions and contaminated soil (Avilés, Spain). The results obtained from the batch mode adsorption studies of Cd ions fitted well with the Langmuir isotherm, and monolayer adsorption capacity of the manganese dioxide-loaded zeolite was about 18 mg/g. The kinetic studies showed that the adsorption of Cd followed the pseudo-second-order kinetic model, which testifies to a chemisorption process. The synthesized nanocomposite adsorbent based on manganese dioxide-loaded zeolite exhibited chemical stability and high efficiency in removing Cd ions from contaminated soil, indicating its great potential for soil remediation.

**ACKNOWLEDGMENTS**

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# Spectroscopic and Structural Characterisation of Zirconia Nanopowders with Multicomponent Stabilization for Energy and Environment Application

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**Abstract ID #NEE-1119**

Zirconia ($ZrO_2$) is a versatile material that possesses unique mechanical, electrical, thermal, and optical properties, making it suitable for a wide range of applications (high-temperature and corrosion-resistant coatings, radiation detectors, biological labeling, catalysts, oxygen sensors, and solid-oxide fuel cells). For many critical applications, $ZrO_2$ with tetragonal and cubic structures is most preferable. For this purpose, $ZrO_2$ doping with subvalent elements is usually applied to stabilize tetragonal and cubic structure via formation of additional oxygen vacancies required for impurity charge compensation. As a consequence, ionic conductivity can be enhanced. At the same time, to achieve high catalytic activity, the powders should demonstrate also developed grain surface covered with catalytically active substances. The production of such powders is a challenging since simultaneous doping with several impurities is used and their interaction cannot be ruled out. Thus, the investigation of the effect of dopant loading and thermal treatment on the structure and spatial dopant distribution is important for obtain high ionic conductivity and catalytic activity of $ZrO_2$-based nanopowders.

In this work, $ZrO_2$-based powders doped with several subvalent elements (such as Y and Cu, Y and Sm, Sc and Ce, Eu, Yb and Y, etc...) were prepared by co-precipitation route followed by the calcination at 400-1100 °C. Besides, these powders were used to produce ceramic samples at 1200-1500 °C. The total dopant content in the powders was 10-11 mol.%. Both powders and ceramics were investigated by means of UV-Vis diffuse reflectance, FTIR reflection spectroscopy, XRD, TEM, Auger spectroscopy and EPR methods. It turned out that among different nanopowders investigated, the most attractive results were obtained for those doped simultaneously with Y, Eu and Yb. These powders demonstrated cubic structure and significant amount of additional oxygen vacancies contrary to the powders singly doped with rare-earths. Besides, the ceramic sintered at 1400 oC showed the highest ionic conductivity that can be attractive for future SOFC application.

It was also found that the $ZrO_2$ doped with Y and Cu showed also significant amount of oxygen vacancies. However, powders with 0.2 - 1.0 mol.% of Cu, calcined at moderate temperatures (600-700 °C) exhibited tetragonal grains with highest surface area covered dispersed CuxO species. It was found that monitoring of Cu spatial localization can allow to predict catalytic activity of the powders and to achieve high rate of the CO conversion in CO-PROX reaction in a wide temperature range (up to 500-600 °C). Our results alsdo showed the utility of complementary spectroscopic methods for the monitoring of the characteristics of $ZrO_2$-based powders with multicomponent stabilization that can give a hand for the non-destructive express characterization of such materials during production process.

**ACKNOWLEDGMENTS**

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# Polylactide Composites with Calcium-containing Fillers

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**Abstract ID #NEE-1121**

Today, more attention is paid to the use of biodegradable polymer materials from renewable raw materials. The most promising is polylactide (PLA) – a biocompatible biodegradable thermoplastic polymer material. Among the methods of directed influence on the morphology and properties of polylactide, the most promising is the development of composite materials based on it with fillers of various nature.

Polylactide Ingeo 2500 HP and nanofillers: calcium orthophosphate and calcium hydroorthophosphate were used in the work to obtain polylactide composite materials. The content of fillers is up to 10 % wt.

The supramolecular structure of polylactide significantly depends on the conditions of its processing and the presence of low molecular weight additives. Also, the crystallization process of polylactide is affected by the nature of the isomers from which it is composed. The conducted studies show that pure PLA crystallites are typical orthorhombic or pseudo-orthorhombic crystals. It was found that the highest value of the degree of crystallinity (46%) is characteristic of the heat-treated sample of polylactide material, and the lowest, respectively, for the original unfilled polylactide (22%).

It was found that the nature of thermomechanical curves of polylactide materials depends on the supramolecular structure of the polymer, as well as on the nature and content of fillers. Thermomechanical curves of polylactide composites, regardless of the nature of the nanodisperse filler, are characteristic of polymers with a partially crystalline structure. The transition to the viscous flow state of PLA-based composites occurs at 190-193 °C. The highest values of the melting temperature of the obtained materials are characteristic of the filled heat-treated samples, which are characterized by the highest degree of crystallinity. One of the significant disadvantages of polylactide materials is low heat resistance, which significantly reduces the potential areas of application of such materials. The introduction of calcium-containing nanofillers slightly increases the Vicat softening point of the developed materials. At the same time, additional heat treatment significantly affects the value of Vicat softening point, in particular, an increase by 40-50 °C is noted. The results of studies of the surface hardness of polylactide materials confirm the effect of calcium phosphates and additional heat treatment on the structure of polylactide. Additional heat treatment contributes to a significant increase in the surface hardness of polylactide composites, regardless of the nature of the filler. The same type of influence of the filler on the value of surface hardness is observed, regardless of the nature of the acid residue of calcium contained in the filler.

The obtained polylactide composite materials filled with calcium can be used to obtain biocompatible implants, biodegradable packaging, and used in 3D printing.

# Development of Nanostructured-Carbon-Supported Silver Nanoparticles and Reduced-Graphene-Oxide-Based Hybrid Supports for Gold and Platinum Catalysts Active at Low Loadings during Oxygen Reduction

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**Abstract ID #NEE-1125**

There has been growing interest in the field of oxygen electroreduction, particularly with respect to potential applications in the science and technology of low-temperature fuel cells. Obviously, many efforts have been made to develop suitable alternative electrocatalysts efficient enough to replace electrocatalysts based on scarce strategic elements such as platinum-group metals. Despite intensive research in the area, there are still a number of fundamental problems to be resolved, and the practical oxygen reduction catalysts still utilize systems based on platinum.

The present study refers to a novel and unique approach of fabrication and deposition of different sized and shaped gold and silver nanoparticles on different carbon supports: carboxylated-graphene, SiO2-doted reduced-graphene-oxide (Gr/SiO2) and chemically reduced graphene oxide. Among important issues is application of inorganic (rather than organic) capping ligand, heteropolymolybdate or heteropolytungstate to modify and stabilize (as well as probably also to link with the oxygen or hydroxyl groups on graphene surfaces) gold or silver nanoparticles. During operation in alkaline medium or neutral media, polyoxometallates disappear but catalytically highly active gold and silver of different shapes remains and exhibit excellent stability. The resulting materials have occurred to show highly potent electrocatalytic properties toward electroreductions of oxygen in alkaline solution. The major advantage of the proposed chemical synthetic method is the integration of the superb properties of both silver nanoparticles and graphene supports in a single-step synthesis with a 100% usage of the silver precursor (AgNO3) according to the coupled plasma mass spectrometer (ICP-MS). What is even more important is that both carbon nanotubes and graphene have occurred to act effectively as carriers for gold and silver nanostructures. Mutual activating interactions are feasible. The conclusions are reached on the basis of diagnostic electrochemical (e.g. rotating ring disk voltammetry), spectroscopic (FTIR) and microscopic (SEM, TEM) experiments.

A series of comparative experiments with different carbon carriers and model catalytic materials (e.g. Vulcan-supported platinum) have also been performed. With respect to oxygen reduction, our diagnostic experiments at different concentrations of H2O2, support a view that the effect of the fast following chemical (H2O2-reductive-decomposition) reaction could be the dominating factor in explaining the observed positive potential shift observed during the oxygen reduction. The fact, that the optimum graphene-based catalytic system produced the oxygen reduction peak current comparable to that observed at the model platinum containing catalyst, would imply the efficient four-electron-type reduction mechanism.

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# Synthesis of Zeolite from Fly Ash Microspheres for Environmental Protection

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**Abstract ID #NEE-1128**

Coal fly ash is a significant industrial by-product, with only 25 % of the total produced being utilized with a low-value-added economic approach, such as wallboard, concrete, and bricks [1]. The remaining 75 % becomes landfill waste, posing a significant environmental concern. Therefore, it is important to find ways to increase the utilization of this waste material to reduce its impact on the environment. One of the by-products of the operation of thermal power plants is fly ash microspheres (FAM), which are gas-filled spherical particles of ash with a lower density than water, making them easy to separate when wet [2]. Furthermore, their distinctive spherical design and chemical composition, which closely resembles that of low-modulus zeolites, make them a promising candidate for zeolite production.

In this study, zeolite (z/FAM) was synthesised by depositing the zeolite phase on the surface of FAM. For this, a selected fraction of FAM was filled with a sodium aluminate solution in a 1:10 solid/liquid phase ratio. The synthesis was carried out at 90 °C for 5 hours, with stirring. At this stage, selecting the optimal mixing speed is important to maintain the material's original spherical shape. Next step, the sample was rinsed with distilled water to achieve a neutral pH, which was controlled using a pH meter, and then dried at 105 °C. It is worth noting that during synthesis, FAM serves not only as a matrix for creating new material but also as an additional source of Al and Si.

Confirmation of the successful completion of the process of obtaining the zeolite phase was carried out by comparing the phase composition of FAM and z/FAM. Scanning electron microscopy (SEM) with energy dispersive X-ray spectroscopy (EDS) was used to study the morphology, size, and shape of microspheres before and after treatment with sodium aluminate solution, as well as to determine the chemical composition of these samples. The characteristics of the porous structure were determined using the method of low-temperature nitrogen adsorption-desorption. The adsorption capacity of the samples was evaluated on the example of the removal of cationic forms of heavy metals (Cu2+). The equilibrium concentration of copper was determined by the inductively coupled plasma atomic emission spectroscopy.

The obtained results indicate that modified samples retain a hollow spherical structure with an average particle size of 172.2 μm and have a secondary outer zeolite layer in the form of thread-like balls (~2-2.5 μm). As a result of FAM zeolitisation, the specific surface area increases by more than 10 times, and the number of pores and their total volume also increase. Compared to the original fly ash microspheres, the z/FAM sample effectively removes copper ions in the pH range from 3 to 6 (75-95%), while the maximum degree of removal for FAM is observed only at pH 6 (68%).

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# Investigation of Optimal Reactor Conditions for Methane Pyrolysis on Gamma Alumina-Supported Fe/Ni Nanoclusters

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**Abstract ID #NEE-1137**

Advanced materials development for clean energy production and utilization, is essential to meet ambitious EU goals and introduce hydrogen energy as one of the gears for the circular economy and GHG emission reduction. Methane pyrolysis offers a cost-effective production of hydrogen from methane by direct conversion avoiding carbon dioxide emissions associated with conventional methods. This method uses already easily available methane feedstock to generate high-purity hydrogen, contributing to the transition towards cleaner energy systems. However, an effective catalyst and appropriate reaction parameters are essential to decrease the activation energy and enhance kinetics and hydrogen yield while minimizing the formation of by-products.

This study shows optimal reaction parameters and the composition of gases produced during methane pyrolysis on novel Fe/Ni nanocluster catalysts supported by gamma alumina [1,2]. It is found that by modifying the catalyst ratio, performing a material and system pre-treatment, optimising measurement methodology, it is possible to decrease the reaction temperature by 200 ℃. In addition, gas analysis demonstrates a hydrogen concentration increase; the carbon deposits on alumina in various forms. The fine-tuning of parameters and modification of catalysts such as ratio and purity underscore the critical role of precisely defined processes in advancing innovative technologies. Our future efforts are focused on obtaining sustainable gamma alumina from aluminium waste, utilizing bio-methane as a hydrogen source, and investigating the potential of residual carbon as a raw material for various use-cases. The general aim is to establish sustainable processes that contribute to clean energy solutions aligned with circular economy principles.

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# Performance Analysis of Turbulent Convection Heat Transfer of $Al_2O_3$-water Nanofluid in the Heat Exchanger of a Water Storage Tank

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**Abstract ID #NEE-1143**

Nanofluids obtained by adding solid nanoparticles to a base fluid significantly improve heat transfer and hydrodynamic flow [1, 2].

In this study, we numerically investigate the convective heat transfer of a turbulent flow inside a U-shaped heat exchanger located in a vertical water storage tank. The water is heated by a U-shaped heat exchanger with tubes Ø 25× 2 mm for 7 hours from a temperature of 5 °C to 50 °C with a variable wall temperature under turbulent flow conditions. The heating fluid is a water-Al2O3 nanofluid with a nanoparticle concentration of 0.1 to 1.3 % vol. The heat transfer efficiency of nanofluid heating compared to water heating is analyzed. The forced motion of the heating fluid with a Reynolds number in the range from 14500 to 18500 was modeled. The simulation results showed that the heat transfer coefficient and Nusselt number increase with the volume concentration of nanoparticles. Compared to the base fluid, the maximum value of the heat transfer coefficient for the water-Al2O3 nanofluid occurred at a volume fraction of Al2O3 of 1.3 %. In this case, the heat transfer coefficient increases by 13 %..

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# Environmental Insight into Efficient Removal of Diclofenac Sodium from Aqueous Solution by $Fe_3O_4$ loaded Mg,Fe-LDH nanocomposites

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**Abstract ID #NEE-1147**

As one of the most typical types of pollutants, pharmaceuticals are acknowledged as one of the most severe environmental pollutants that adversely affect humans and aquatic organisms due to their widespread application, biological intractability, and toxicity. According to partial statistics, nearly 10,000 tons of drug stuff in annual use originate from the pharmaceutical/medicine industry, and more than 30% of its drug stuff is discharged into the water stream. Diclofenac sodium (DCF) and Ibuprofen are some of the most common drugs used in modern medicine. It possesses inherent toxicity, carcinogenicity, and mutagenicity. It had been proved that DCF could not readily biodegradable. The current technologies for the removal of organic pollutants include advanced oxidation, photocatalysis, electrochemical degradation, coagulation, and adsorption. Adsorption technology has been widely used for the removal of pharmaceuticals to its advantages of a wide range of raw materials.

In this work, Fe3O4 loaded Mg,Fe-layer double hydroxides (Mg,Fe-LDH×xFe3O4, x = 0 to 0.5) nanocomposites were prepared via the in-situ growth of Mg,Fe-layered double hydroxides (LDHs) onto magnetite nanoparticles and applied for anionic DCF motives removal. These materials are prepared by a combination of co-precipitation and hydrothermal methods, and systematically characterized by several techniques e.g. X-ray diffraction (XRD), Scanning electron microscopy with energy dispersive X-ray spectroscopy (SEM/EDX), Vibrating sample magnetometer (VSM), Transmission electron microscope (TEM), etc.

The XRD patterns confirms formation of both LDHs and magnetic phases. The plate-like morphology is evident by TEM confirm Mg,Fe-LDH, and Mg,Fe-LDH×xFe3O4 nanocomposite. The layered-like morphology is evident by SEM. VSM and SEM/EDX confirm magnetic nanocomposites. Higher Fe3O4 loading leads to an increase in the hydrodynamic sizes of the nanocomposite structure. Various influence factors like concentration, pH, and time were systematically investigated. The maximum adsorption capacity for Mg,Fe-LDH×0.3Fe3O4 was 158.16 mg/g. Further results indicated that the adsorption isotherm for diclofenac anions retention could be fitted to Freundlich and Langmuir equations. The values obtained indicate that organic groups are adsorbed on Mg,Fe-LDH by an electrostatic process, hydrogen bonding, and complexation reactions, but without a significant anion-exchange process. Besides, after 3 regeneration cycles, Mg,Fe-LDH×0.3Fe3O4 still retained high ordered morphology with a magnetic response.

**ACKNOWLEDGMENTS**

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# Light Scattering by Black Silicon Layers

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**Abstract ID #NEE-1172**

Black silicon (b-Si) comprises needle-like surface nanostructures where the needles are made of single-crystal Si. These needles enhance light absorption rather than reflecting it back from the surface. The combination of low reflectivity and the semiconductive properties of Si found in b-Si make it an ideal candidate for application in solar cells as frontal antireflection surfaces [1]. However, while the primary focus typically lies on studying total light reflection and absorption, investigating light scattering by the b-Si layer is equally significant. Such an analysis will enable us to delve deeper into the optical behavior of b-Si and choose appropriate encapsulation materials for solar modules.

This study investigates total light reflection and scattering by b-Si layers formed using reactive ion etching. The corresponding spectra were determined in the visible, near-infrared, and near-ultraviolet wavelength ranges (250–1400 nm). It is demonstrated that the presence of b-Si layers results in decreased reflectivity and increased scattering across the entire spectral range of interest. Increasing the etching duration strengthens this trend. However, b-Si layers cannot be considered perfect scatterers due to a monotonic decrease in the diffuse reflectance coefficient at wavelengths greater than 600 nm.

The possibilities of using b-Si layers in solar cells and photodetectors are discussed.

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# Pseudocapacitive TiO2 as an Efficient Decoupled Electrolysis Mediator in Acid

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**Abstract ID #NEE-1183**

Decoupled electrolysis has proven to be a novel method for safe hydrogen production, but improvement is still possible. Redox mediators allow us to produce $H_2$ and $O_2$ in separate time and space, avoiding explosive gas mixtures. A critical factor in developing new redox mediators is the availability of the material and non-toxicity. Traditionally used acidic solid-state redox mediators are $V_2O_5$, $WO_3$ and $MoO_3$, but they are relatively scarce and unavailable in the EU; that is why developing new materials, in this case- $TiO_2$, is essential. Here, we demonstrate a decoupled electrolysis system with $TiO_2$ quantum dots of 4.5 nm as an efficient redox mediator in acidic electrolytes. $TiO_2$ nanoparticles showed a high electrochemical surface area on carbon felt supported, with a specific capacity of 375 F/g, ten times larger than commercially available $TiO_2$ $P_{25}$ nanoparticles. During the $O_2$ production cycle, $H^+$ ions intercalated in the $TiO_2$ redox mediator, forming $Ti^{3+}$, as demonstrated by XPS results and observable colour change. Produced electrodes showed high stability even after 3000 cycles with an overall energy efficiency of 52.4% and gas purity above 98%. These results demonstrate the perspective of $TiO_2$ as a possible alternative to well-established redox mediators for decoupled electrolysis. Decoupled electrolysis with cheap and abundant redox mediators can provide a viable alternative to membrane electrolysers, eliminating the need for expensive membranes and extensive pressure-equalising systems.

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# Synthesis and Optical Properties of Pr-doped $K_2O$-$B_2O_3$-$P_2O_5$-$Bi_2O_3$ Glasses

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**Abstract ID #NEE-1209**

The light emission diodes (LEDs) are considered as the best devices for lighting applications. Theoretically, LEDs possess the highest electricity-to-light transformation efficiency and long operation time. However, due to degradability of polymer (silicone) binder under action of high temperatures and light fluxes, the LEDs undergo significant loses in intensity and color properties of emission.

Luminescent glasses and glass-ceramics have attracted significant attention recently as alternative for commonly used light converters for LEDs base on silicon substrate [1]. In case of white LEDs such converters should absorb an ultraviolet or blue emission from semiconductor chip and emit in /green/orange/red regions. Some rare-earth ions in various glass or crystalline hosts have been considered as suitable for suchlike applications, and $Pr^{3+}$ ions are among them owing to orange/red luminescence [2]. It is worth noting a luminescence of the host usually remains out of consideration because of its low intensity except specific cases of glasses/crystals with luminescent moieties, e.g. $MoO_4$ groups or $Bi^{3+}$ ions.

In present study the Pr-doped $K_2O$-$B_2O_3$-$P_2O_5$-$Bi_2O_3$ glass system has been obtained by conventional melt quenching technique. It was found, that BiPO4 micro/nanocrystals can be formed in the glass body if cooling procedure is not fast enough. Thus, glass-ceramics can be formed by spontaneous glass crystallization. The obtained samples have been characterized by means of optical microscopy, X-ray powder diffraction, IR absorption, diffuse reflection, and photoluminescence (PL) spectroscopies. The density, molar volumes, band gap values and color characteristics of the studied glasses were estimated.

The XRD patterns of the samples consist exclusively of wide bands, those are typical to amorphous phase. IR analysis indicated a presence of some phosphate groups, e.g. $P_2O_7$ ones. The photoluminescence of the samples highly depends on excitation conditions. In particular, excitation in the 430-500 nm range results in intensive $Pr^{3+}$ relatively wide band emission with maxima near 600 nm. Such wideband emission indicates that praseodymium ion occupies a site in the amorphous phase of the sample. The studied glasses reveal also own emission consisting of three wide bands with maxima near 450, 600, and 700 nm. An intensity of each band depends strongly on glass composition.

The studied luminescent glasses can be considered as perspective materials for further elaboration of nanostructured optical glass-ceramics for white LEDs applications.

## ACKNOWLEDGMENTS

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# Exploring Gas-Metal Alloy Nano-Interfaces for Developing Self-powered Devices and Sustainable Applications

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**Abstract ID #NEE-1212**

Gas-metal interfaces present unique prospects across various engineering domains, encompassing nanofilm synthesis for electronics and sustainable engineering applications. In electronics, these interfaces enable the synthesis of sensors, transparent nano-field effect devices, ferroelectric memory devices, and nanogenerators. They also support sustainable practices such as direct carbon dioxide capture and reduction to valuable products, along with advancements in energy storage technologies.

This presentation delves into the research surrounding the utilization of near room temperature processed solid and liquid alloys for these purposes. Metal alloys serve as efficient solvent catalysts for nanomaterial synthesis in electronics and energy utilization applications, while also facilitating the synthesis of green chemicals as catalyst materials. Additionally, they offer atomically thin interfaces crucial for environmental remediation technologies.

Metals and metal alloys interact with gases to generate atomically thin interfaces that can be synthesized and harvested for various applications. Understanding the preferred reactions of elements in specific phases and morphologies on the surface of metal alloys and interfaces is fundamental to this process, governed by the Gibbs free energy of reaction.[1] Through this methodology, nanofilms and interfaces can be synthesized.

Nanofilm materials directly harvested from surfaces of liquid Tellurium alloys [2] and solid Titanium metal [3] surfaces exhibit enhanced p-type performances, showcasing promising materials for transparent electronics and high mobility atomically thin transistors. Furthermore, utilizing the latest liquid metal synthesis method of instant-in-air liquid metal printing process with liquid bismuth results in the formation of naturally occurring, air-stable, atomically thin, mechanically flexible nanogenerators and ferroelectric oxides. [4]

Despite challenges related to symmetry disruption, nanogenerator devices demonstrate polarization switching, which is measured and utilized for ferroelectric nanopatterning. These liquid alloy interfaces offer versatility, providing unique and dynamic nanointerfaces for energy and catalyst applications. The presentation concludes by highlighting and expanding the nanointerfaces for sustainable engineering practices, such as room-temperature CO2 capture and conversion to solid carbon, [5] as well as the development of super capacitor layers [6], underscoring the versatile prospects of near room temperature metal alloys in gas atomically thin interfaces.

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# Characterization of Direct p-n Junctions in Layered Zinc Oxide-Copper Oxide Nanowire Heterostructures

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**Abstract ID #NEE-1215**

The operating principle of many devices such as diodes, thermoelectric generators (TEGs), and solar cells is based on a p-n junction between adjoined p-type and n-type semiconductors [1,2]. In an effort to utilize materials which are more environmentally friendly and safer for general use, the properties of zinc oxide (n-type) and copper oxides (p-type) are actively being explored, and higher efficiency materials and structures are still being developed. Our previous research on these materials has proven especially promising, concerning the fabrication of TEGs [3,4]. Nanostructuring has helped to increase their efficiency and reduce their size, but fabricating a direct p-n junction between the materials would increase the effective surface area and improve electrical contact, whilst eliminating the need for an insulating material between the p-type and n-type material, which is often a part of a typical TEG layout. To utilize the benefits of a direct p-n junction for the application in TEGs, a new heterostructured material is proposed by depositing a zinc oxide layer directly on a copper oxide nanowire array.

The morphology and electrical properties of the zinc oxide-copper oxide nanowire heterostructure were characterized based on the synthesis parameters of copper oxide nanowires and zinc oxide to copper oxide ratio in the heterostructure. The copper oxide nanowire arrays were synthesized at different oxidation temperatures and varied amounts of zinc oxide was deposited on top of the copper oxide nanowires. It was found that the integrity and morphology of copper oxide, synthesized at different oxidation temperatures, affected the material's electrical properties. A p-n junction was observed during electrical measurements of different regions of the heterostructured material, where the copper oxide to zinc oxide ratio varied. The study of synthesis parameters' effect on the morphology and electrical properties of zinc oxide-copper oxide heterostructures provides a useful insight for the further development of materials with a direct p-n junction, which could be used in TEGs or other devices based on such structures.

## ACKNOWLEDGMENTS

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# Dissipation of Current Carriers in Lead Telluride Films

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**Abstract ID #NEE-1221**

Lead telluride films are promising materials for detectors and sources of infrared spectrum of optical radiation. The mechanisms of current carrier scattering have an important influence on the operational characteristics of device structures based on them [1]. The dependence of the mechanisms of current carrier scattering in thin polycrystalline PbTe films on the thickness (2.5-7.7) microns in the temperature range (77-300) K has been studied.

In thin films, the following occurs: scattering on the crystal lattice in the bulk of the film, surface, and growth defects [2]. PbTe films for the study were prepared from the vapor phase using the hot wall method onto glass substrates. The film growth rate was 1-3 nms-1. The structure of the films was studied by electron microscopy and diffraction, as well as optical metallography. The electrical parameters of the films were measured using the compensation method in constant electric and magnetic fields. The measurements were carried out on separate films of different thicknesses. The current through the samples was 0.1 mA. The magnetic field was directed perpendicular to the surface of the films at an induction of 0.8 T. The sample being measured had two current and four Hall contacts.

The thickness dependences of electrical conductivity, Hall coefficient, charge carrier mobility, and carrier concentration for PbTe films were studied. It has been established that with increasing film thickness there is an increase in the specific electrical conductivity, as well as the mobility of charge carriers and the value of the Hall coefficient. In this case, the Hall concentration of current carriers decreases.

An expression is obtained for calculating the mobility of current carriers in thin films during scattering on the surface and in the intergrain limits. The dependences of current carrier mobility for PbTe films deposited on glass substrates on thickness and temperature have been studied. It is shown that the dominant mechanism is carrier scattering at grain boundaries. The thickness dependences of the current carrier mobilities of PbTe films, calculated for scattering at grain boundaries, differ slightly from the experimental ones, which further confirms the dominance of current carrier scattering at grain boundaries. The activation energy of electrical conductivity associated with scattering at grain boundaries is estimated.

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# Membranes via Atomic Layer Deposition for Energy and Environmental Uses

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**Abstract ID #NEE-1254**

Atomic Layer Deposition (ALD) stands out as a cutting-edge technology enabling the fabrication of thin films using high-quality materials on substrates with high aspect ratios. This technique offers precise control over thickness, uniformity, and outstanding conformality, making it particularly suitable for modifying the structure and customizing the pores of highly porous materials such as synthetic membranes. ALD coatings have been successfully applied to a wide range of membrane substrates, from inorganic templated supports to porous polymers.

In this presentation, we aim to offer a thorough overview of the advancements made in utilizing ALD on highly porous materials, specifically those employed in membrane technology. Leveraging a thoughtfully selected array of our research endeavors, we will illustrate how ALD can effectively enhance the operational efficiency of various membrane types, including inorganic, organic, hybrid, or composite membranes. Through exemplification, we will highlight the pivotal role of ALD in crafting membranes with precisely tunable geometries, facilitating systematic exploration of the correlation between physical-chemical properties and geometric parameters. This approach enables comprehensive investigations into membrane performance across diverse applications, encompassing areas such as renewable energy, including gas separation and osmotic energy harvesting, as well as environmental applications like water treatment and sensor technologies.

Additionally, we will address the challenges and prospects associated with integrating ALD into membrane applications. This presentation endeavors to provide a comprehensive overview of the advantages of ALD and its applications across various aspects of membranes and related engineering processes. It aims to illuminate the numerous opportunities within this burgeoning and rapidly advancing field.

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# Multi-element Modulation of High Entropy Spinel-structured Oxides as Innovative Phtocatalysts for Energy Conversion

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**Abstract ID #NEE-1267**

High configurational entropy and the synergistic interactions among multiple cations mixing emerged to an promising class of materials as called high-entropy oxides [1,2]. These mixed oxides incorporate multiple mettalic cations into a single crystalline phase, resulting in novel and unexpected properties [3,4]. The present study focuses on the synthesis and characterization of single spinel oxide phase consisting of six different metallic cations Co-Fe-Ni-Mn-Zn-Cu for applications in photocatalytic water oxidation process. We developed a rapid and low-temperature synthesis method involving precipitation in a highly alkaline medium at 90°C, resulting in the formation of high entropy spinel-structured oxide phases. Structural, morphological, optical and magnetic properties of the synthesized samples were comprehensively assessed through a vast variety of complementary characterization techniques such as powder X-ray diffraction analysis (XRD), field-emission scanning electron microscopy (FE-SEM), ultra high-resolution transmission electron microscopy (UHR-TEM) and X-ray photoelectron spectroscopy (XPS). Additionally, the magnetic properties were determined by vibrating sample magnetometry (VSM). Structural characterization using X-ray diffraction (XRD) and Rietveld refinement confirmed the formation of a cubic spinel structure with Fd-3m symmetry and the successful incorporation of six different transition metal cations (Co2+, $Fe^{2+}$, $Ni^{2+}$, $Mn^{2+}$, $Zn^{2+}$, $Cu^{2+}$). The results demonstrated that the high-entropy configuration imparts enhanced stability and catalytic properties. This work highlights the potential of High Entropy Spinel-structured Oxides as efficient and stable photocatalysts, paving the way for further research and development in sustainable hydrogen production.

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# Evaluation of a Polymer Composite Material for Application in Microbial Three Electrode System

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**Abstract ID #NEE-1275**

The global energy demand is exponentially surpassing the rate of energy generation leading to scarcity of fossil fuelswhile giving rise to greenhouse gas emissions. But the requirement for renewable and cost-efficient technologies led the research towards biological systems to reduce environmental pollution and recover valuable resources. Among biological systems, bio-electrochemical systems (BES) are significant sources for treatment of wastewater, energy generation and clean fuel production incorporating Microbial fuel cells (MFCs) for electricity generation and Microbial electrolysis cells (MECs) for production of hydrogen and methane gas [1]. In the present work, polymer-based electrode was developed for BES using dip coating technique. Polymer composite is prepared with a blend of polyaniline as a conductive polymer and polystyrene as a base material which acts as a medium of contact with the substrate. This polymer-based electrode was operated as working electrode in a single chamber microbial three electrode system. Performance of the system is evaluated using chronoamperometry (CA) where a maximum current of 120µA was obtained through this process with Shewanella oneidensis as the model electrochemically active bacterium. Current has increased up to 200µA by introducing CNT nanoparticles into the polymer composite [2]. The concentration of the polymer and the number of dips required to form layer by layer assembly was optimized based on the characteristics of the electrode developed. Surface morphology of the electrode and interaction of microbes with the electrode surface was characterized for identifying the structural features using FESEM. Due to its cost effectiveness, the energy generated through this system can be used as power sources in bio-batteries, biosensors and other applications [3].

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# Reduced $TiO_2$ based kHz supercapacitor for AC line filtering application

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**Abstract ID #NEE-1276**

An electrolytic capacitor, generally an Aluminium electrolytic capacitor (AEC), is widely used for applications such as ripple-current filtering, high power, power conversion, load levelling, and pulsed power generation. However, AEC is the bulkiest component because of the low areal capacitive behaviour, which is a limiting factor for downscaling portable devices or circuit boards. A high-frequency response supercapacitor can work at a kilohertz frequency higher than 3-4 orders than traditional electrochemical capacitors, and it can replace the AEC [1-2].

TiO2 is one of the best candidates in the metal oxides category due to its natural abundance, environmental friendliness, and low cost. TiO2 nanotubes provide high surface area and vertically homogenous morphology. Titanium dioxide has attracted immense interest in applications such as dye-sensitized solar cells, batteries, supercapacitors, photocatalysis, sensors, and biomedical devices [3]. However, TiO2 nanotube electrode material has not been investigated extensively for the application of supercapacitors as an AC line filter.

So, in this work, we investigated and developed a titanium-based electrochemical capacitor by electrochemical anodization followed by an electrochemical reduction method with enhanced capacitance and phase angle at 120Hz comparable with the best carbon-based supercapacitor, which helps to replace the bulky AEC for line-powered electronics. It exhibits a high electrode areal capacitance of 1030 μFcm-2 and a phase angle of -82.2° at 120 Hz with a characteristic frequency of 1.675 kHz. Additionally, it shows a Resistor-Capacitor (RC) time constant of 167.7 μs. The practical application of our reduced TiO2 NTAs supercapacitor for AC line filtering demonstrates its promising capability to replace AEC in compact devices. The upper frequency limit of the operation for the pseudocapacitor, as measured by the self-resonance frequency was a high value of 80 kHz.

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# Synthesis of $Fe_3O_4$ Magnetic Nanoparticles on Modified Multi-Walled Carbon Nanotubes for Laccase Immobilization and Its Potential Application in the Degradation of Emerging Pollutants in Wastewater

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**Abstract ID #NEE-1280**

The COVID-19 pandemic has led to a significant 32% increase in the prescription of antidepressants, with alprazolam (VFX) emerging as a prominent contaminant. This has underscored the urgent need for sustainable alternatives in pharmaceutical waste management. Biological treatments utilizing enzymes such as laccase have shown promise, boasting elimination rates of up to 70%. However, challenges persist in terms of stability and reusability of these enzymes. To address these issues, we focused on enhancing laccase immobilization using advanced materials like multiwalled carbon nanotubes (MWCNT) and magnetic nanoparticles (MNP). These materials have demonstrated remarkable immobilization efficiencies, reaching up to 100%, and have shown reusability for up to 16 cycles for other emerging contaminants.In our investigation, we synthesized magnetic MWCNT (mMWCNT) through co-precipitation in two different molar proportions: 1:1 MWCNT:MNP (system A) and 1:0.5 MWCNT:MNP (system B). Our goal was to evaluate the impact of molar variation on immobilization efficiency and pH stability, using laccase from the regional Pycnoporus sanguineous CS43 strain. Characterization of the materials was conducted through Fourier-Transformed Infrared Spectroscopy, X-ray diffraction, Zeta potential measurement, and TEM imaging.Our results revealed that system B exhibited a higher immobilization efficiency of 93.2% compared to system A (83.0%). Additionally, system B demonstrated a higher ζ-potential, indicating improved stability across a wider pH range, unlike system A, which was stable primarily in the pH 4-5 and 7 range. This optimized immobilization system was further applied to successfully biodegrade alprazolam, showcasing its potential as an effective and eco-friendly approach to treating pharmaceutical waste.

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# Removal and Recovery of Dissolved Oil from High-Salinity Wastewater Using Graphene–Iron Oxide Nanocomposites

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**Abstract ID #NEE-1283**

Produced water (PW) is a major byproduct of oil and gas extraction, posing significant environmental risks due to its oil contamination. Traditional methods for removing dissolved oil from PW are often inefficient, especially in the presence of high salinity. Graphene-based nanocomposites offer a promising solution due to their high surface area and tunable properties. This study investigates the synthesis and application of a reduced graphene oxide-iron (III) oxide nanocomposite (rGO-$Fe_2O_3$-NC) for dissolved oil removal from high-salinity wastewater.

The rGO-$Fe_2O_3$-NC was successfully synthesized and characterized. Batch and column adsorption experiments demonstrated exceptional oil removal efficiency exceeding 90% within 30 minutes, even under short contact times. The maximum adsorption capacity, determined by the Langmuir model, reached an impressive 1301 mg/g. Remarkably, the adsorption performance of the nanocomposite was enhanced in high-salinity conditions (up to 100,000 ppm), highlighting its suitability for PW treatment. This enhanced performance in saline conditions may be attributed to a salting-out effect [1].

The adsorption kinetics followed a pseudo-second-order model, indicating a chemisorption-driven process. Regeneration studies using ethanol demonstrated that the rGO-$Fe_2O_3$-NC maintained over 80% adsorption capacity through three cycles, illustrating good recyclability. Compared to other graphene-based adsorbents, including those used for general oil-water separation [2], the rGO-$Fe_2O_3$-NC exhibited superior performance offering a potentially cost-effective and sustainable solution.

This study underscores the potential of graphene-iron oxide nanocomposites [3] for efficient dissolved oil removal from high-salinity wastewaters. Future research directions include optimizing the nanocomposite's structure and exploring its applicability in real-world PW treatment scenarios.

## ACKNOWLEDGMENTS

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# Charge Transfer in the Fe/g-$C_3N_4$/$MoS_2$ Heterojunction: a Computational Study

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**Abstract ID #NEE-1285**

Hydrogen production via solar-driven water splitting with the aid of catalysts is currently a topic of immense research. Photocatalysts based on two-dimensional (2D) semiconductors have exhibited exceptional efficacy compared to conventional counterparts. In particular, graphitic carbon nitride, g-$C_3N_4$ is a prominent 2D photocatalyst with wide a band gap conducive to visible light absorption, high specific surface area, and abundant active sites [1]. Nonetheless, the rapid recombination of the photogenerated electron-hole pairs undermines the photocatalytic efficiency of g-$C_3N_4$. Designing 2D/2D van der Waals heterojunctions based on g-$C_3N_4$ is an effective strategy to remedy this limitation, facilitating swift charge separation through the hetero-junction and thereby enhancing the photocatalytic performance [2]. Furthermore, achieving superior performance of the hetero-structure relies on the precise control of the interfacial region of the hetero-junctions. In this study, we demonstrate, using density-functional calculations, that the interfacial charge transfer can be finely modulated by embedding transition metal atoms in the g-$C_3N_4$/ $MoS_2$ heterostructure. Our findings reveal that introducing a Fe atom can either augment or diminish the charge flow between the g-$C_3N_4$ and $MoS_2$ layers, contingent upon its spatial positioning. The direction of the induced electric field between the layers can be predicted through the computation of their respective work functions. These findings could help elucidate the experimentally observed enhancement in photo-catalytic performance of g-$C_3N_4$/ $MoS_2$ heterojunctions [3]. They also offer valuable guidance for the rational design of superior photocatalytic heterostrucures.

## ACKNOWLEDGMENTS

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# Functionalized Porous WS2 Nanostructures for Improved Performances in Hydrogen Evolution Reaction and Photovoltaics

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**Abstract ID #NEE-1310**

We have recently investigated porous inorganic chalcogenides nanostructures for various sustainable energy related applications, in particular as hydrogen storage media, in photovoltaics for enhancement of the perovskite solar cells efficiency, and as electrocatalysts for hydrogen evolution reaction (HER).

Significant research endeavours have been dedicated to the search for highly efficient and cost- effective electrocatalysts for the HER. WS2 nanotubes were previously demonstrated for electrocatalysis performances owing to their unique chemical structure and physical properties. We report here a new method of surface modification through cold radiofrequency (RF) plasma. The effect of two plasmatic ions ($D_2^+$ and $Ar^+$) on $WS_2$ nanotubes has been investigated. The plasma-treated samples showed improved performances in HER electrocatalysis due to interaction of plasma ions with pores and impurities in the nanopartciles surface and their intercalation in between the atomic layers. In particular, it induced formation of the surface and subsurface oxide layers responsible of the electrocatalytic improvement. Based on experimental results, both Ar and $D_2$ plasma treatments, when performed separately, show similar effects on electrocatalysis performances with improved HER overpotentials of 348 and 343 mV at -10mA/cm2 compared to 567 mV of the pristine $WS_2$ nanotubes. On the other hand, combined treatment by Ar and then by D2 radio frequency plasma notably decreases the overpotential to 264 mV.

Perovskites materials attract much attention due to their high photoluminescence quantum yield and versatile chemical processability nature. However, light, thermal effects, moisture and chemical reactions with oxygen lead to their degradation and such perovskite solar cells (PSC). Herein, we are working to overcome the instability of PSCs by developing the novel hybrid perovskite/$MS_2$ nanocomposites for PSCs. $MS_2$ (M = W or Mo) nanotubes are capable of absorbing a wide range of visible light and are very stable. Combining $MS_2$ nanotubes and perovskites can increase the stability of so produced composite. As MS2 nanotubes support polaritonic modes at room temperature, they are optically active in Vis and NIR-IR regions and so can be exploited for light absorption and emission across this spectral range. Such composites might offer an additional benefit of charge transfer. For this purpose, they are exposed to focused ion beams to induce Ga atoms implantation aiming to improve their electrical conductivity and decrease the band gap.

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# Peculiarities of Ion Transport in Aqueous Electrolytes Confined in Anodic Alumina (AAO) Nanochannels

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**Abstract ID #NEE-1318**

Nanofluidics has received increasing attention in the field of energy conversion in recent years. Various unique ion transport properties within nanochannels, including selective ion transport, ion current rectification, and ion concentration polarization, have been exploited to develop energy-harvesting devices. The ion transport can be caused by various driving forces, such as external pressure gradients, electrostatic forces, temperature, or concentration gradients. Thus, understanding the transport behavior of electrolyte solution through nanochannels is crucial to increasing the energy-conversion efficiency.

Porous anodic alumina (AAO) is characterized by self-assembled straight cylindrical nanopores produced by electrochemical oxidation, making it particularly attractive as a material for nanofluidic platforms. The diameter and length of nanochannels can be varied by choosing optimal synthesis parameters. The pore walls are also available for further functionalisation, which makes it possible to use AAO membranes as fundamental materials for the preparation of various nanocomposites.

In this work, ion transport within AAO nanochannels was studied, and the impact of the nanoporous platform structural parameters, the charge of the nanochannels` internal surface, and the type/concentration of the electrolyte on ion behavior in the solution was determined. For the current study, AAO membranes were fabricated using the two-step anodisation method in a 0.3 M sulfuric acid electrolyte. The nanochannels were infiltrated with aqueous electrolytes (NaCl, $NaClO_4$, $Na_2SO_4$) in the concentration range from $3 \cdot 10^{-5}$ M to 1 M using the hydrostatic pressure-induced method. The infiltration of nanochannels was controlled by electrochemical impedance spectroscopy (EIS). To determine the stability of AAO membrane in an aqueous electrolyte solution the morphology of the membranes before and after infiltration was examined using scanning electron microscopy (SEM). The dependence of ζ-potential values, determined by pressure-driven ion transport, on the charge of the nanochannel walls and solution pH, was established. Moreover, the changes in the electrolyte solution filtration rate were used to indicate the occurrence of nanoconfinement effects or damaging/degradation processes in AAO pore channels.

# Thermoelectric Properties Of Aqueous Electrolyte Infiltrated In Anodic Aluminium Oxide (AAO) Nanochannels

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**Abstract ID #NEE-1320**

The direct conversion of heat to electricity without any intermediate steps remains one of the most auspicious, yet challenging, methods of power production, especially due to the ongoing global decarbonisation trend. Moreover, due to the wide variety of readily available heat sources, such as the combustion of fossil and other fuels, nuclear reactors, solar heat, or even waste heat recovery from the human body and household appliances, the applications for thermal-to-electric energy converters are broad. The development of a new nanofluidic platform technology based on the ion transfer in nanofluidic membranes would lead to a breakthrough in versatile and sustainable energy harvesting and storage. To achieve this goal, the formation of nanochannels through rational design is required. Fabrication of perfectly engineered nanofluidic membranes is critical to generate a substantial thermovoltage, i.e. high ionic Seebeck coefficient, in the presence of a temperature gradient, by confining ion transport in charged nanochannels.

Nanoporous anodic aluminum oxide (AAO) is one of the most popular and cost-effective platforms for various applications: from templates and molecular separation to drug delivery and energy generation. AAO membranes have highly ordered nanochannels and offer the opportunity to precisely engineer the morphology of nanochannels.

In this work, a nanofluidic platform based on 25 nm-pore AAO membranes with a thickness of 50 microns was fabricated and infiltrated with $Na_2SO_4$ aqueous electrolyte to implement ion transport and energy generation by converting electrokinetic and thermal energy into electricity. The sandwich-type cell was initially designed to test the thermoelectric properties of aqueous electrolyte-infiltrated AAO membranes. Applying a temperature difference to the system revealed an increase in output voltage attributed to thermally driven ion transport in the nanochannels, which tended to decrease with increasing concentration. The dependence of output voltage per Kelvin obtained from ion thermodiffusion inside the nanofluidic membrane on electrolyte concentration could be used to investigate the contribution of electrokinetic effects that occur in nanochannels and are especially noticeable when electrical double layers along the inner walls of the nanopores are completely or partially overlapped.

# Metal Oxides-Based Nanostructured Hybrid Materials for Mitigation of Climate Changes

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**Abstract ID #NEE-1326**

Energy consumption, and in particular the burning of fossil fuels, is the main source of human-induced greenhouse gas emissions, resulting in climate change and decreasing air quality. But at the same time, energy is also a fuel for economic growth. The challenge that the world is facing now is how to maintain economic growth while reducing the carbon content of energy and increasing the efficiency of its use. Generating green energy from renewable sources as solar energy and/or heat (photovoltaic/thermoelectrical devices) are among the fastest technologies to roll out and meet these targets.

Recently, zinc and copper oxides have attracted considerable attention because of their promising potential to contribute to an energy-efficient society. These materials exhibit remarkable photo- and thermoelectrical properties and are low-cost, abundant, and non-toxic. At the same time, these materials in the form of powder are commercially used for photo- and thermocatalytic $CO_2$ reduction.

This work presents recent developments in the application of nanostructured zinc and copper oxide-based materials for low-grade waste heat harvesting and approaches combining photovoltaic/thermovoltaic and photothermocatalytic technologies in self-powered multifunctional materials/devices for simultaneous energy generation and $CO_2$ reduction.

Zinc oxide (ZnO), copper oxide (CO), and hybrid ZnO-CO nanostructures and nanostructured networks were synthesized using thermal evaporation, physical vapour deposition, and thermal oxidation methods. The investigation methods included electron microscopy, energy-dispersive X-ray spectroscopy, X-ray photoelectron spectroscopy, X-ray diffraction technique, in-plane and cross-plane electrical, photo/thermoelectric, and photo/thermocatalytic characterization in gaseous environment. The effect of structure, morphology, and chemical composition of the synthesized oxide nanostructure on energy harvesting and photo/thermocatalytic properties is discussed.

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# Synthesis of Pd@Au@ZnO Double Core-Shell NPs with Different Pd and Au Composition and Their Optical Properties

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**Abstract ID #NEE-1355**

Metal@MOS(metal oxide semiconductor) core–shell structure composite nanoparticles (NPs) have attracted considerable attention as a means to design novel structures that are different from their single component counterparts [1–4]. The morphological structure and optical properties of these core–shell structure nanoparticles (CS-NPs) can be maintained even at high temperatures because the coalescence of the core material and the crystal growth of the shell materials are greatly restricted. Therefore, these core–shell composite nanoparticles have potential applications in optical processing, advanced coatings, photocatalysis and gas sensing.

Au NP is a typical plasmonic material and can be used in optical and catalytic applications. On the other hand, Pd NP does not show a plasmonic phenomenon but exhibit excellent catalytic applications. Combining noble metal core NPs with other metals can improve the optical and catalytic properties of the MOS shell [5].

In this study, we synthesized Pd@Au@ZnO double CS- NPs to create new materials for optical and catalytic applications. For synthesis of Pd@Au@ZnO double CS-NPs, we first prepared Pd@Au CS-NPs with different compositions by controlling Au shell thickness (1, 3, 5, and 7 nm), and then formed Zn(OH)2 outer shell using hydrothermal method. These double CS-NPs were heat-treated at 500ºC for formation of ZnO outer shell. The morphologies, crystal structures and core compositions were observed using SEM, HR-TEM, XRD and XPS, and the optical properties were investigated using UV-vis spectrometer in detail.

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# Elastic Topological Insulator/Carbon Nanotube Heterostructures for Green Energy Harvesting

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**Abstract ID #NEE-1370**

Topological insulators (TI) are materials with dominant surface conductivity, where charge carriers are protected from scattering. Due to their unique combination of properties, TIs have attracted great interest for applications in various fields, ranging from quantum computing to thermoelectric generators and effective electrodes for energy storage devices. To fully exploit the unique properties of TIs, the material should be downsized to a nanometer scale to suppress its bulk conductance.

A classic representative of topological insulators are bismuth and antimony chalcogenides (Bi2Se3, Bi2Te3, Sb2Te3), layered narrow-band gap semiconductors, which also possess remarkable thermoelectric properties at near-room temperatures. In this work, a cheap and easy-to-implement physical vapor deposition method was used for the synthesis of various heterostructures, which are formed by combining topological insulators with different carbon allotropes as p-type and n-type single- or multiwalled carbon nanotubes alone or combined with C60 molecules or MXenes.

In such heterostructured materials, chalcogenide nanostructures synthesized on top of CNTs provide direct electrical and mechanical contact between them, stabilizing the heterostructures during bending and improving charge transfer between the heterostructure components. Flexible generators made from polymer-encapsulated heterostructures are 2-4 orders of magnitude more efficient than generators made from other thermoelectric materials based on non-conducting polymers. Moreover, Bi2Se3-based heterostructures containing n-type CNTs were found to be more thermoelectrically efficient compared to one based on p-type CNTs. For the deep insight into the charge transfer mechanisms, resulting in such a remarkable improvement of properties, resistance and magnetotransport measurements of heterostructures composed of different components in different wt.% ratios were performed in the temperature range 2-300 K and analyzed.

TI-CNT and TI-CNT/MXene heterostructures showed superior performance also as binder-free electrodes for their applications in Li and Na ion batteries, providing stability during expansion/contraction associated with the charge and discharge processes and additional ion accumulation possibilities. In addition, the Bi2Se3-CNT network was found to be a highly selective catalyst for CO2 reduction to methanol in a gaseous environment, operating under natural sunlight without the need for an external power source.

TRACK 12

# “NANOBIOMEDICAL RESEARCH & APPLICATIONS”

# Mimicking Neuroligin-2 (NL-2) Function in Pancreatic $\beta$-cells by Nanocomposites as a Novel Approach for Antidiabetic Therapy

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**Abstract ID #NRA-0919**

Both pancreatic $\beta$-cell membrane and presynaptic active zones of neurons are the assembly sites of similar protein complexes mediating regulated secretion of bioactive molecules. These synapse-inducing proteins include neuroligins and their binding partners: neurexins. These proteins participate in trans-cellular protein-protein interactions across the synaptic cleft. It was shown that $\beta$-cells express both neuroligins and neurexins on their plasma membrane. It was also found that insulin secretion and the proliferation rate of $\beta$-cells increased when $\beta$-cells were co-cultured with cells overexpressing neuroligins. We propose that neuroligin-derived molecules arranged in clusters can enhance $\beta$-cell function and functional maturity, as well as protecting $\beta$-cells in stress conditions. To test this hypothesis, several peptides were derived from crystal structures of different neuroligins and neurexins using molecular modelling methods. These peptides were conjugated with nanoscale composites. Covered by NL-2 derived peptide nanocomposites (HSA-28D) enhanced $\beta$-cell functions in terms of glucose-stimulated insulin secretion and protects them under stress conditions in vitro and ex vivo. [1-3]. Recruiting the $\beta$-cells' "neuron-like" secretory machinery as a target for diabetes treatment is a novel approach. Such nanoscale composites might therefore provide a unique starting point for designing a novel class of antidiabetic therapeutic agents and "artificial $\beta$-cells" development.

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# Mesenchymal Stem Cells as Delivery Vehicles of Nanoparticle-Photosensitizer Complexes to Cancer Cells

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**Abstract ID #NRA-0922**

Mesenchymal stem cells (MSCs) have attracted much attention as therapeutic carriers due to their inherent capacity to migrate to tumor sites. Buddhadev Layek et al. showed that the accumulation of cargo within MSCs does not alter their tumor-homing potential [1]. However, the cargo needs to be carefully selected to ensure that the controllable release of active compounds happens only after the MSCs reach tumors and not before. One of the ways to control the activity of the cargo – is to use light-activated materials – photosensitizers (PS). In the absence of light, PS has no toxicity. Once PS molecules absorb light of an appropriate wavelength, they initiate photocytotoxic reactions in the area of its presence (i.e., photodynamic therapy). The limitation of such a therapy is the shallow tissue penetration of visible light. To reach the deeper layers of tumors, nanoparticles (NPs) must be employed as energy donors to extend the excitation spectrum of PS molecules [2].

In this study, we used complexes of rare-earth-doped upconversion nanoparticles (RENPs) and photosensitizer chlorin $e_6$ (RENPs-$Ce_6$) to create the MSC-based delivery vehicle (MSCs-Nano-Vector). MSC-Nano-Vector proved its migratory abilities and selectivity to cancer cells. The RENPs-Ce6 cargo did not alter the viability of MSCs, and surprisingly, increased the migration efficiency of MSCs when loaded with the complex compared to empty MSC vectors. Co-cultures of MSCs and cancer cells revealed that 2-step irradiation with 980 nm laser induced death of both MSCs and cancer cells via singlet oxygen-induced phototoxic reactions.

In our study, we proved the concept of MSCs employment in the targeted delivery of nanotherapeutics to cancer cells to be valid for RENP-$Ce_6$s cargo. Further studies are needed to understand the behavior and therapeutic efficacy of MSC-Nano-Vector in more complex biological models.

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# Skin Mesenchymal Stem Cells and Upconverting Nanocomplex for Two-Step Photodynamic Therapy

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**Abstract ID #NRA-0924**

Cancer remains a global health challenge, and the main treatment methods lack effectiveness and specificity, causing adverse effects. One of the less aggressive treatments is photodynamic therapy, but current photodrugs (e.g. chlorin $e_6$ ($Ce_6$)) are activated by visible light, which has a low penetration through the tissues and affects only superficial tumours. Therefore, nanoparticles that can be used as diagnostic agents and photodrug carriers are being developed. Among these nanoparticles are upconverting nanoparticles (UCNPs), which are non-toxic, photostable, and with excitation and emission in the optical tissue transparency window, allowing them to be used not only for tumour diagnostics but also for therapeutic applications when linked with photodrug. These nanoparticles can be excited with near-infrared radiation ($\lambda_{ex}$ = 980 nm or 793 nm) resulting in emission in the visible part of the spectrum. As a result, the photodrug $Ce_6$ attached to the nanoparticles is excited and can generate singlet oxygen, that is cytotoxic and leads to cell death [1]. However, only a small fraction of nanoparticles reach cancer cells due to their low specificity, dense intracellular matrix, and macrophage impact [2]. To overcome this problem, we have used mesenchymal stem cells (MSCs) as upconverting nanocomplex carriers, due to their ability to migrate towards the tumour upon chemokine stimulation. In our studies, we have shown that upconverting nanocomplex accumulates in MSCs and is biocompatible. Also, we have demonstrated that MSCs can transport this complex to cancer cells. Finally, our results showed that irradiation with 980 nm laser excitation has a significant phototoxic effect on nanocomplex-loaded cells in cell monolayer and spheroid models using two-dose irradiation. Overall, our results demonstrated that active upconverting nanocomplex transportation using MSCs could increase the efficiency of photodynamic therapy.

## ACKNOWLEDGMENTS

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# Graphene Quantum Dots with Excitation-Wavelength-Independent Photoluminescence under Multiphoton Excitation: Nitrogen Functionalities in Dual-Modality Near Infrared–I/II Bioimaging and Photodynamic Therapy

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Doping sorted graphene quantum dots (GQDs) with heteroatoms and functionalizing them with amino acid could improve their radiative recombination and two-photon properties—including their excitation-wavelength-independent photoluminescence from the ultraviolet to the near-infrared-I (NIR-I) region, absorption, quantum yield, absolute cross section, lifetime, and radiative-to-nonradiative decay ratio—under two-photon excitation (TPE) at a low excitation energy and short photoexcitation duration, as determined using a self-made optical microscopy system with a femtosecond Ti–sapphire laser. Four types of sorted GQDs were investigated: undoped GQDs, nitrogen-doped GQDs (N-GQDs), amino-functionalized GQDs (amino-GQDs), and N-doped and amino-functionalized GQDs (amino-N-GQDs). Among them, the sorted amino-N-GQDs are effective as a two-photon photosensitizer and generate the highest quantity of reactive oxygen species for the elimination of multidrug-resistant cancer cells through two-photon photodynamic therapy (PDT). Larger amino-N-GQDs result in a greater number of C–N and N–functionalities, leading to a superior photochemical effect and more favorable intrinsic luminescence properties, making the dots effective contrast agents for tracking and localizing cancer cells during in-depth bioimaging in a three-dimensional biological environment under TPE in the NIR-II region. Overall, this study highlights the potential of large amino-N-GQDs as a material for future application to dual-modality two-photon PDT and biomedical imaging.

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# Chlorin $e_6$ Localization in the Coating of Upconverting Nanoparticles: Theranostic Realization

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Cancer remains one of the leading causes of death worldwide. In 2024, it is estimated that over 1.2 million deaths from cancer will occur only in European Union [1]. The introduction of nanotechnology and nanoparticles into the biomedical field offers opportunities to create biocompatible, theranostic nanoplatforms with adjustable properties. Theranostics is a term used to characterize the combined therapeutic and diagnostic tasks performed by a single system; therefore, it can eliminate multi-step medical procedures, reduce delays in treatment, improve patient care, and provide early diagnostics. Furthermore, theranostics has led to more accurate cancer diagnosis and treatment.

In this context, Chlorin $e_6$ ($Ce_6$) functions as a photosensitizer which, when loaded in the phospholipid/polyethylene glycol (PLPG)-coated upconverting nanoparticles (UCNPs), creates a theranostic nanoplatform. As a result of UCNPs exceptional emission properties, UCNPs serve in cancer diagnostics, while $Ce_6$ is responsible for the generation of singlet oxygen for photodynamic therapy (PDT).

This study aimed to identify the placement of Ce6 in the PLPG coating on $NaGdF_4:Yb^{3+},Er^{3+}@NaGdF_4:Yb^{3+},Nd^{3+}$ rare earth UCNPs. Hydrogenated soybean phosphatidylcholine (HSPC) and 1,2-distearoyl-sn-glycero-3-phosphoethanolamine phospholipids conjugated with polyethylene glycol (DSPE-PEG) were applied for the investigation. Spectroscopy results revealed, that $Ce_6$ emission and absorption peaks shift and vary depending on the type of PLPG covering the UCNPs, indicating different placement and interaction sites of Ce6 with the PLPG of UCNPs. Oleic acid, used to coat UCNPs after synthesis, provides one site of attachment, while PLPG offers a biocompatible coating with additional site for the interaction with $Ce_6$. Additionally, it is well known, that PEG plays a crucial role in extending the nanoplatform's circulation half-life when introduced into the bloodstream. We anticipate that the developed nanoplatform will serve as a promising candidate for targeted drug delivery and effective cancer therapy. By altering the phospholipid coating, we can manipulate the placement of $Ce_6$ within the nanoplatform, thus modulating its overall properties. This research not only enhances our understanding of photosensitizers but also contributes to the broader comprehension of nanoplatforms in cancer therapy.

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# MXene-GNRs Nanocomposite Incorporated Injectable Hydrogel for Photo-Chemotherapy of Cancer

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Cancer is a major cause of death globally, prompting extensive research for new treatment methods. In 2020, there were over 19 million documented cancer cases and one million deaths, underlining the need for effective treatments [1]. Nanomedicine offers promising solutions for cancer therapy due to its improved selectivity, minimal side effects and ability to convert light into heat due to photothermal effect and thus can be explored as drug delivery vehicle. Photothermal therapy involves heating of tumor region to several degrees above the physiological temperature (37 °C), and thus recently has been explored against cancer with the help of nanotechnology in synergy with chemotherapy through controlled anticancer drug release [2]. Additionally, the light-to-heat conversion properties of MXene nanomaterials have propelled their significance in cancer therapy [3]. Gold nanorods, for their selective light absorption and heat generation capabilities, also stand out as effective photothermal agents. Alongside, the emergence of injectable hydrogels as versatile drug carriers in cancer treatment adds a compelling dimension. Integrating nanomaterials within these hydrogels not only reduces systemic side effects but also enhances treatment efficacy through controlled, localized hyperthermia induction, enabling precise tumor targeting [4].

The current study investigates the integration of MXene-GNRs nanocomposite with pH and thermoresponsive injectable hydrogel for triggered release of paclitaxel, a commonly utilized chemotherapeutic agent. Using the photothermal properties of the nanocomposite, main objective is to enhance drug release control, thereby improving the therapeutic outcome in cancer treatment. The approach involves synthesizing the MXene-GNRs nanocomposite particles and embedding these within an injectable hydrogel matrix, followed by comprehensive assessment of its photothermal properties. Overall, the results illustrate that the MXene-GNRs nanocomposite exhibits a superior photothermal response compared to individual nanoparticles. Moreover, near-infrared (NIR) irradiation, performed in two ON/OFF cycles, effectively triggers controlled release of paclitaxel under acidic conditions (pH 5.0), resulting in approximately 47% release compared to around 10% release without NIR irradiation. Additionally, at pH 7.4, NIR irradiation leads to approximately 32% release of paclitaxel compared to less than 10% release without NIR irradiation over three hours, thereby highlighting the potential for on-demand drug delivery. This study underscores the promise of MXene-GNRs nanocomposite-integrated hydrogels in enhancing paclitaxel delivery via photothermal effects, thus advancing nanotechnology-based strategies for cancer treatment.

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# Leveraging Omic Biology for the Advancement of Cancer Nanotherapies

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**Abstract ID #NRA-0946**

In the realm of cancer nanotherapeutics, nanomaterials have emerged as promising platforms for drug delivery due to their unique properties such as targeted delivery, prolonged circulation, and stimuli-responsive drug release. These nanotherapeutic agents have showed their potential in cancer treatment by enhancing drug efficacy, minimizing side effects, and improving patient outcomes [1]. However, cancer arises from a complex interplay of genomic aberrations, including mutations, copy number alterations, expression changes, and epigenetic modifications across multiple omic layers [2]. Therefore, in order to design much effective treatment modalities for the clinic, we need to consider the biology behind these nanosystems. This talk delves into the integration of omics data in the nanomedicine field to enhance the understanding and efficacy of cancer nanotherapeutics. The utilization of 'omics' technologies, including metabolomics, genetics, metagenomics, transcriptomics, and proteomics, offers a comprehensive approach to unravel the intricate relationships between tumor cells, tumor microenvironment and nanomaterials. Our group has used various omic approaches to reveal the mechanisms behind various cancer nanotherapeutics including carbon dots, quantum dots and 2D materials including MXenes [3-6]. The talk will underscore the importance of harnessing omic biology to propel cancer nanotherapeutics forward, ultimately improving patient outcomes and revolutionizing cancer care.

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# Stable PEG-Silver Nanoparticles Biomaterial for Medical Applications

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Lately, nanomaterials have been studied as innovative alternative solutions for classical procedures. Able to overcome many challenges regarding the final properties of a material, nano-biomaterials are evolving every day, receiving more consideration due to their nano sizes and their versatility. Among their industrial, chemical or pharmaceutical applications, their medical purposes proved to be important markers in the development of efficient nano systems for soft tissue engineering and antimicrobial applications. The implementation of non-toxic and biocompatible nanomaterials able to offer support while assuring faster healing is the key for an ingenious strategy.

Silver nanoparticles (Ag NPs) are considered metallic nanoparticles with high efficiency in biomaterials fabrications based on their antibacterial effect [1]. Ag NPs can be synthesized in the laboratory for antibacterial and antioxidants effects using various chemical techniques. One of the most important properties is related to their size, therefore a clear physical analysis of this characteristic can be correlated with their ability to inhibit bacteria multiplications [2,3]. In this work, silver nanoparticles aqueous solutions were synthesized using a friendly method with a low-cost process starting from a nitrate salt and poly (ethylene-glycol) (PEG). To increase their biocompatibility and their stability, PEG-Ag NPs polymer system was proposed since the association with PEG will improve nanoparticles' surfaces and will control Ag NPs sizes for further medical applications.

The found in the PEGylated Ag NPs compared to Ag NPs were confirmed by the changes in Fourier-Transform Infrared Spectroscopy (FT-IR) and UV-VIS spectra where distinctive peaks were observed. The dimensions were identified using Dynamic Light Scattering (DLS) and Atomic Force Microscopy (AFM). Furthermore, the analysis showed different values in the case of the system proposed, so a more uniform size distribution was achieved. The PEG-Ag NPs nanomaterial proved to have proper characteristics for its medical application, so it can be considered an innovative nano-biomaterial.

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# Biomedical Properties of Nano-modified Nerve Conduits

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Recently, there has been an increase in the number of cases of nerve tissue damage caused by both physical injury and congenital defects, such as cancer. As a result, more than 100,000 nerve replacement procedures are performed annually in European countries. Engineered nerve conduits are a modern alternative to the use of autografts and allografts. The development of conduits capable of conducting nerve impulses at the level of human nerves, while maintaining biological inertia relative to the human body, has been the major challenge in this field in recent years.

To ensure high electrical conductivity, multicomponent nanocomposites containing graphene oxide nanoparticles ($GO_{NPs}$) and carbon nanotubes (CNTs) have been developed.

CNTs- and $GO_{NPs}$-based nanocomposites [1] have been widely reported for their applications in tissue engineering. Among conductive materials, $GO_{NPs}$ have shown excellent conductivity and mechanical strength, which have significant effects on the stimulation, proliferation, and differentiation of neural stem cells [1].

Studies have shown that all prepared composites have sufficient hydrophilicity (contact angle ~ 46-66$^{o}$) to attach somatic cells. Rat brain neurons, after isolation and transplantation, adhered to the plastic and formed a monolayer, with most of the cells adhering. In the experimental samples, adhesion was slightly reduced at the border of the neural conduit. When analyzing the MTT data, a decrease in the intensity of the reaction in the presence of $GO_{NPs}$-containing neural conductors is observed. This means that nanoparticles with a concentration of 150 μg/ml have little effect on cell survival.

Antimicrobial studies showed no activity of the CNTs- and $GO_{NPs}$-based nanocomposites against Gram-negative bacteria *E.Coli* ATCC-25922 and a more significant effect against Gram-positive *S.Aureus* ATCC-25923 (ZOI 12.5 and 13.3 mm, respectively).

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# $TiO_2$ Nanoparticles with the Varying $Ti^{4+}/Ti^{3+}(Ti^{2+})$ Ratio EXacerbate TBOOH-Induced Oxidative Stress

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$TiO_2$ nanoparticles are promising agents in the biomedical field. In particular, accumulating evidence indicates that $TiO_2$ nanomaterials can be potentially applied as anti-cancer agents. Cancer cells are known to show elevated basal levels of reactive oxygen species (ROS), and ROS induction by nanotechnology-based approaches is a widely applicable strategy for anti-cancer treatment. In this study, we demonstrated the ability of three $TiO_2$ nanoparticles with the different ratios of stoichiometric ($Ti^{4+}$) and non-stoichiometric ($Ti^{3+}$ and $Ti^{2+}$) titanium ions in their crystal lattice to aggravate tBOOH-induced ROS production in L929 cells. Flow cytometry-based 2',7'-dichlorodihydrofluorescein diacetate (H2DCFDA) staining revealed that the percentage of non-stoichiometric $Ti^{3+}$ and $Ti^{2+}$ ions in the crystal lattice of $TiO_2$ nanoparticles might affect the degree of tBOOH-induced oxidative stress. Notably, $TiO_2$ nanomaterials did not affect basal ROS production in L929 cells at the concentrations that promoted tBOOH-induced ROS overproduction. Our findings suggest that modulation of stoichiometric ($Ti^{4+}$) and non-stoichiometric ($Ti^{3+}$ and $Ti^{2+}$) titanium ions in the crystal lattice of $TiO_2$ nanoparticles may modify their redox properties affecting anti-cancer capacity.

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# In vivo Application of 3D-Bioprinted Scaffolds with MXene Quantum Dots in Breast Tissue Regeneration after Mastectomy

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**Abstract ID #NRA-0972**

Breast cancer stands as one of the most prevalent malignancies affecting women [1]. Managing the risk of cancer recurrence and facilitating the regeneration of breast tissue post-surgical interventions are pivotal for effective breast cancer treatment [2]. Recent advancements offer promising outcomes in breast tissue regeneration post-breast cancer [3]. Notably, various tissue scaffolds have been shown to be effective in cancer treatment, which incorporates nanomaterials via 3D-bioprinting [4]. However, surgical procedures like mastectomy and therapies such as radiotherapy and chemotherapy lead to cancer recurrence, permanent tissue damage, and aesthetic concerns, substantially impacting patient well-being. Here, we demonstrate the effect of hydrogel-based 3D-bioprinted scaffolds with MXene quantum dots (MQDs) transplanted in vivo after mastectomy in rat and mouse models of breast cancer on inhibiting tumor recurrence and promoting breast tissue regeneration. In the in vitro and in vivo analyses of our study, we observed high CK14 and TGF-$\beta$ expression in the acellular collagen-based 3D-bioprinted scaffold group 14 days after transplantation. Furthermore, the absence of tumor recurrence in this group resulted in superior tissue regeneration compared to other groups. Increased CK14 production and high TGF-$\beta$ expression, which are important in breast tissue remodeling and indicate the presence of basal epithelial cells, indicate tumor suppression, cellular participation in the healing process, and accelerated new tissue formation [5]. Our findings suggest that 3D-bioprinted MQD-containing scaffolds can serve a dual role by supporting surgical intervention for regeneration and averting tumor recurrence. This approach holds promise as a viable and innovative treatment modality for breast cancer in the future. We anticipate that our developed nanomaterial-containing 3D scaffold could emerge as an innovative material applicable to various cancer types, including breast cancer. Moreover, it presents alternative perspectives by contributing to regeneration, potentially eliminating the need for chemotherapy and radiotherapy following cancer surgery.

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# Macroporous Filtration PTFE Membranes Modified with Polymer-Based Nanocomposite Containing Zirconium Hydrophosphate and Silver Nanoparticles

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Membrane filtration is promising and cost-effective technology of separation. The most limitation of membrane methods is undesirable fouling phenomenon caused by deposition of colloidal particles, macromolecules, proteins and inorganic species [1]. Two beneficial methods are used to prevent the membrane fouling - development of the membrane hydrophilicity and adding antibacterial agents to the membrane Such approaches include the modification of membranes with advanced carbon nanomaterials [2, 3], inorganic ion exchangers [4], or their composites [5], as well as silver nanoparticles [6]. The plane membranes are usually used for this purpose. But the efficiency of their work depends not only on the pressure, but also on the geometric parameters of the membrane modules. As opposed to plane materials, the efficiency of tubular polymer membranes, for instance, microfiltration polytetrafluoroethylene (PTFE), can be controlled by regulation of their length. The disadvantages of these materials are low separation ability as well as fouling with organic substances. Here we show a possibility of the transformation of microfiltration separator into ultrafiltration membrane by means of its modifying with a multicomponent composite containing polymer (to provide the most complete filling pores), zirconium hydrophosphate (for rigidity of polymer tube and also for hydrophilization) and silver nanoparticles (for antibacterial properties). Silver nanoparticles were prepared by different methods and their antibacterial activity was tested against Gram-positive and Gram-negative bacteria. It was established highest antibacterial activity for silver nanoparticles synthesized from the plant extract (green biosynthesis) They showed inhibition in following row: *Candida albicans* > *Pseudomonas aeruginosa* > *Staphylococcus aureus, Escherichia coli* >*Salmonella spp*. The advantages of biosilver nanoparticles include biocompatibility and eco-friendly synthesis conditions. The most promising samples of bio silver nanoparticles were incorporated into polymer-inorganic nanocomposite following modification tubular PTFE membrane. The selectivity of the membrane towards globular proteins was found to reach 35 % (bowine serum albumin, 69 kDa) 57 % (ovalbumine, 32 kDa), and 42 % (lactalbumine, 15 kDa) at low pressure (0.5 bar). indicating the. Thus, it indicates transformation of microfiltration material to ultrafiltration membranes separator with antifouling properties. The modified membranes can be recommended for water and wastewater treatment, and also for needs of food and beverage industries.

## ACKNOWLEDGMENTS

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# The Upconverting Nanoparticle Emission Quenching by Water in Different Cell Culture Media

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**Abstract ID #NRA-0986**

Upconverting nanophosphors gathered interest in numerous applications. The upconversion (UC) luminescence efficiency is known to be nanoparticle size-dependent [1]. The lanthanide ions inside the "core only" nanophosphors and those on the surface can show different emission intensities because the surface dopants are more prone to surface quenching effects [1, 2]. Therefore, decreasing the size of upconverting nanoparticles (UCNPs) to sub-10 nm levels decreased the UC luminescence. We have studied the temperature transformations of the magnetic centers on model organometallic nanosystems – metalloorganic complexes and conjugated polyarenes doped with magnetic nanoclusters. Investigation of the magnetic center dynamics was carried out on powder samples, sealed in quartz ampules, using the EPR spectrometer of the X-ray range in the temperature interval of 4.2-300 K.

The size dependent UCNPs emission originates from phonon-mediated energy transfer processes, [4] surface effects related to high energy vibrations of ligands, surfactants [2, 3], from increased surface defect density, [1, 2] and surrounding solvents [1] containing OH-, CH-groups, small biomolecules and serum proteins.

To use UCNPs in nanobiomedicine they must be rendered water dispersible [4]. Several strategies have been devised to enhance UC luminescence: inert outer shell addition, optimizing ion concentrations, and introducing organic molecules to improve light absorption or energy conversion efficiency. In addition, the aqueous environment can impact the UCNPs' UC emission and stability [2].

In this work, colloidal stability and UC quenching by environment of $LiYF_4$: $Yb^{3+}$, $Tm^{3+}$ nanocrystals in different aqueous solutions as water, phosphate buffer, cell growth media DMEM and OptiMEM were detected. In media full of salt, amino acids, small biomolecules, proteins UCNPs cover themselves instantly with a biomolecular shell that repels water molecules further away from the surface. Therefore, the water sensing is minimized, and the emission and stability of UCNPs is maximized.

Drastically different UC emission intensity changes were detected in DMEM and OptiMEM supplemented with fetal bovine serum. Addition of proteins increased stability due to corona formation on the nanoparticle surface that repels water molecules from the surface and cause smaller water quenching [5]. Furthermore, proteins in media not only stabilize the UCNPs but are partially responsible for cellular uptake.

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# Effect of $TiO_2$ Nanoparticles Defect Structure on their ROS Scavenging Ability

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**Abstract ID #NRA-0996**

$TiO_2$ nanoparticles (TiNPs) have gained considerable attention as agents that can regulate the level of reactive oxygen species (ROS) within cells [1]. TiNPs have been reported to be promising in drug delivery, sonodynamic, photodynamic, photothermal, and ionizing radiation therapies for cancer, as well as antimicrobial and antioxidant agents [1].

In the present report, we have analyzed the effects of TiNPs defect structure associated with the presence of stoichiometric ($Ti^{4+}$) and non-stoichiometric ($Ti^{3+}$ and $Ti^{2+}$) titanium ions in the crystal lattice and TiNPs aggregation state on their ROS scavenging ability in cell-free and $H_2O_2$-treated L929 cells. TiNPs of two types with different amounts of $Ti^{3+}$ and $Ti^{2+}$ ions were synthesized and characterized by XRD, TEM, SAXS, and XPS methods. TiNPs antioxidant properties were analyzed by chemiluminescence and optical spectroscopy methods using ROS sensors. Chemiluminescence and total antioxidant capacity tests indicate the radical scavenging ability of the synthesized TiNPs with a stronger effect for TiNPs with a larger amount of non-stoichiometric Ti ions. Both types of TiNPs were revealed to exert $H_2O_2$ decomposition ability in cell-free medium. It has been demonstrated that the concentrations of TiNPs up to 40 mg/L have no impact on cell viability, cell death, and motility of L929 cells. At the same time, TiNPs neither alleviated nor aggravated $H_2O_2$-induced oxidative stress in L929 cells.

Our findings provide insights into possible mechanisms of TiNPs antioxidant activity.

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# Effect of Hydrogen Peroxide Decomposition on Luminescence and Microstructure of $GdVO_4:Eu^{3+}$ Redox-Active Nanocrystals

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**Abstract ID #NRA-1006**

Hydrogen peroxide plays a crucial role in the functionality of living cells. It acts as a mediator in various physiological processes, impacting cellular metabolism and signaling pathways. Some key functions of hydrogen peroxide in cellular processes include cellular metabolism regulation, cell differentiation and proliferation, immune response, development of various pathologies and even cell death [1].

Sensing intracellular levels of hydrogen peroxide is crucial due to its potential to cause cell mutations and lead to various pathologies. Doped orthovanadate nanoparticles show promise as multifunctional theranostic agents [2] and intracellular hydrogen peroxide sensors [3]. Therefore, detailed studies are required to understand factors influencing their catalytic and luminescence properties, particularly the impact of hydrogen peroxide on their luminescent behavior.

In this study, we investigated the effects of hydrogen peroxide on $Eu^{3+}$ luminescence quenching and microstructure of $GdVO_4:Eu^{3+}$ nanocrystals synthesized in an aqueous solution. The obtained nanocrystals were characterized using X-ray diffraction (XRD), high-resolution transmission electron microscopy (HR-TEM), X-ray photoelectron spectroscopy (XPS), and optical spectroscopy techniques.

To examine surface microstructure modifications of $GdVO_4:Eu^{3+}$ nanocrystals after exposure to hydrogen peroxide, we employed XPS analysis and time-resolved luminescence spectroscopy. Two mechanisms responsible for the observed $Eu^{3+}$ luminescence quenching were identified: reduced efficiency of non-radiative resonance energy transfer from vanadate ($VO_4^{3-}$) groups to $Eu^{3+}$ ions due to reducing of vanadium ions, and direct quenching of $Eu^{3+}$ luminescence by $OH^-$ groups formed on the surface as a result of hydrogen peroxide decomposition.

This study enhances our understanding of how hydrogen peroxide influences the luminescent properties and surface microstructure modifications of $GdVO_4:Eu^{3+}$ nanocrystals, thereby contributing to their potential as effective intracellular hydrogen peroxide sensors.

## ACKNOWLEDGMENTS

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# Enhancement of Thiol Oxidation by Redox Cyclers in the Presence of Nanoparticles in Model System

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**Abstract ID #NRA-1016**

Redox-cycling compounds are widely used in tumor chemotherapy. Such compounds include quinones and ascorbic acid, the antitumor effect of which is synergistic. In this work, inorganic nanoparticles (NPs) based on rare earth elements are used as catalytic amplifiers of one-electron transfer with the formation of organic and oxygen radicals in the redox cycles of ascorbic acid and vitamin K3. As an indicator of the pro-oxidant efficiency of the action of NPs ($CeO_2$ (2 nm, 20 μg/ml) or $GdYVO_4:Eu^{3+}$ (2 nm, 20 μg/ml)) combined with organic compounds (ascorbic acid (100 or 200 μM), vitamin K3 (4 μM)) changes in the level of thiols (glutathione (200 μM), L-cysteine (200 μM) or dithiothreitol (500 μM)) in the model system were used. The pH dependence (pH 6.7; 7.4; 7.8) and time dynamics of the process within 24 hours were studied. It was shown that the presence of orthovanadate and cerium dioxide NPs enhances oxidation of thiols under an influence of each of the redox-cyclers as well as their combination. The efficiency of nanoceria was higher compared to orthovanadate NPs (including time dynamics) that was especially pronounced in the dithiothreitol oxidation system. The data obtained indicate the ability of nanoceria to significantly enhance the oxidation of thiols induced by redox cyclers, which indicates the perspective of this approach in solving the problem of increased thiol level in tumor cells.

# Synthesis and Spectral Properties of New Long-Alkyl-Chain-Modified Flavonols as Fluorescent Probes for Nanostructured Materials

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**Abstract ID #NRA-1020**

Fluorescent probes based on 3-hydroxy-4H-chromen-4-one (3-hydroxyflavone, flavonol) have a wide range of applications in medical and biological research [1-2]. Functionalization of 3-hydroxyflavones by introducing long-chain alkyl anchor groups helps to increase their selectivity and affinity to biological and synthetic macromolecules due to non-covalent binding. For this purpose, we synthesized a series of fluorescent probes based on 3-hydroxyflavone, which contain hydrophobic long-chain alkyl radicals of different lengths (2, 6, 12 carbons) in the 4'-position.

The synthesis of the 3-hydroxyflavone derivatives was carried out by linear or one-step methods, starting from the corresponding substituted aromatic aldehydes and 2-hydroxyacetophenones. Intermediate derivatives of 1-(2-hydroxyphenyl)-3-(4-alkoxyphenyl)prop-2-en-1-one carboxylic acids were isolated and identified separately using a linear method of synthesis. The heterocyclization reaction (Algar-Flynn-Oyamada reaction) was carried out by heating the intermediate 1-(2-hydroxy-phenyl)-3-(4-alkoxy-phenyl)prop-2-en-1-one in methanol with an aqueous solution of potassium hydroxide and peroxide hydrogen [3].

Our synthesized flavonols, when used to study the structure of biological and synthetic macromolecules, revealed significant insights. For instance, the enzyme *β*-glucosidase and polyvinylpyrrolidone were examined in an aqueous solution using fluorescence spectroscopy, molecular docking and molecular dynamic modeling. The introduction of hydrophobic alkyl radicals of a certain length was found to enhance the binding of the probe molecule to the enzyme, indicating a potential for more effective enzyme inhibition. This discovery opens up exciting prospects for creating new *β*-glucosidase inhibitors based on our hydrophobically modified probes [4].

The obtained model and target flavonol derivatives have the synthetic potential for their further modification by introducing functional groups (-OH, -SH, -$NH_2$) for anchoring and functionalizing silver and gold nanoparticles.

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# Antioxidant Complexes Based On Cyclodextrin-Coated Ceria Nanoparticles For Biomedical Applications

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**Abstract ID #NRA-1024**

The diversity of catalytic activities and antioxidant properties of cerium oxide nanoparticles ($CeO_{2-x}$ NPs) makes them promising materials for the theranostics of various diseases, especially those caused by disturbances in free radical homeostasis in living systems. Despite the fact that the functionalization of the surface of nanoparticle plays a critical role in nanomedicine, the effect of different coatings on their enzyme-like behaviour and antioxidant properties is still poorly understood, which limits the biomedical application of $CeO_{2-x}$ NPs.

Here we propose the new method of obtaining beta-cyclodextrin – $CeO_{2-x}$ ($\beta$-CD@$CeO_{2-x}$) complexes with addition of $\beta$-CD on the stage of syntheses of NPs. The combination of nanoparticles (NPs) with antioxidant properties (so-called nanozymes) and hydrophobic antioxidant molecules using CD@NPs complexes can increase sufficiently the antioxidant efficiency of both components due to synergistic effect. As a result, highly stable colloidal solutions of nanometer-size (2–3 nm) $\beta$-CD@$CeO_{2-x}$ nanoparticles were obtained. The results on the antioxidant activity of $\beta$-CD@$CeO_{2-x}$ complexes (determined by luminol chemiluminescence, coumarin oxidation and epinephrine autoxidation) show that $\beta$-CD@$CeO_{2-x}$ complexes are potent as •OH and $O_2^-$ scavengers. $\beta$-CD@$CeO_{2-x}$ complexes are stable in various biological media (glucose solution, Tris, and Hepes), and can be additionally stabilized by FBS in order to prevent their agglomeration in other ones (NaCl, PBS, DMEM, and C199). Antioxidant properties of $\beta$-CD@$CeO_{2-x}$ NPs paved the way for obtaining complexes of water-insoluble antioxidant molecules and $CeO_{2-x}$ antioxidant NPs, for which synergistic antioxidant action of molecules and NPs was observed.

# The Antitumor Efficacy of Redox-Active Inorganic Nanoparticles/Menadione Complexes in 2D AND 3D Models of L929 Fibrosarcoma Cells

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**Abstract ID #NRA-1025**

The oxidoreductase-like activity of nanoparticles, due to their electronic properties, makes it possible to target key processes in cancer cells, including the generation of ROS, the exchange of low molecular weight antioxidants, and the metabolism of energy substrates. There are evidences that the antitumor effect of NPs is enhanced when used simultaneously with redox-active organic compounds. Cholesterol-based complexes of ultra-small (1-2 nm) inorganic orthovanadate nanoparticles ($GdYVO_4/Eu^{3+}$ NPs) or cerium oxide nanoparticles ($CeO_2$ NPs) with menadione were developed to specifically damage the oxidative balance and metabolism of cancer cells. Since the combination of ascorbic acid with menadione is an inducer of autoschizis (specific cancer cell death), the effect of menadione-containing complexes was also studied in the presence of vitamin C. The antitumor efficacy of the complexes was assessed on L929 mouse fibrosarcoma cell line in 2D and 3D models.

Nanoparticles: cholesterol: menadione (1: 0.02: 0.4) complexes were used. In 2D model, L929 cells (~ 2 x $10^4$ cells/ml) were incubated with complexes (NPs - 10 μg/ml / menadione - 20 μmol) in DMEM/F12 with 3% FBS in humidified atmosphere with 5% $CO_2$ with or without vitamin C (2 mmol). In 3D model, 7-days obtained spheroids of L929 cells were used. Fluorescent microscopy with DHE, JC-1, PI, acridine orange and MTT tests were used for the effect assessment.

In 2D experiments, complexes based on $CeO_2$ NPs more effectively inhibited the functional activity of cells in the presence of vitamin C, which was accompanied by cell shrinking (in autoschizis), a decrease in mitochondrial potential, and the formation of superoxide radicals. The time and strength of the destructive action depended both on the concentrations of FBS and complexes. This effect in the 3D model required a three-fold increase in the concentrations of complexes and vitamin C. Three week experiments on the 3D model showed partial inhibition of cell viability at an x1-fold concentration of used compounds and complete destruction of the 3D structure at an x3-fold concentrations. So, unlike 2D model at least a three-fold increase in the active components was necessary in 3D model. It should be considered in evaluation of antitumor efficiency and the development of treatment protocol.

# Design And Research Of Thermo-Responsive Gelatin-Alginate-Humic Nanocomposite Hydrogels For Controlled Drug Delivery

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**Abstract ID #NRA-1047**

The use of biomaterials, including biopolymers, to create "smart" hydrogels is a promising area of modern science and technology [1]. The most widely used biopolymers for this purpose are proteins (silk fibroin and gelatin) and polysaccharides (cellulose, chitosan and sodium alginate), the important features of which are low cost, renewability, biocompatibility and biodegradability [2]. The purpose of this work is to create a bioactive "smart" thermo-responsive gelatin-alginate-humic nanocomposite hydrogel, which, when exposed to the body with a physiological temperature of 37 °C, reversibly turns into a sol, which can be used to introduce drugs into hard-to-reach places, for local and long-term delivery of drugs, as well as for reducing doses of delivered drugs. All design thermo-responsive nanocomposite hydrogels based on the gelatin -sodium alginate-humic acid systems developed to date have melting points below the physiological temperature of 37 °C. Considering the relevance of creating a biocompatible thermo-responsive hydrogels with a physiological melting point based on non-toxic and available biomaterials that have wound-healing properties and are suitable for controlled drug delivery, in this work we developed and studied a more complex gelatin -sodium alginate-humic acid system. The optimization of the compositions of thermo-responsive biologically active gelatin-alginate-humic nanocomposite hydrogels by studying their rheological properties using the viscosimetric method in order to adjust the melting temperature to physiological conditions is done. It is assessment of the temporal conditions of the gel-sol transition of thermo-responsive bioactive gelatin-alginate-humic nanocomposite hydrogels with physiological melting point, and the characterization of these thermo-responsive GN-SA-HAs-$H_2O$ hydrogels using Fourier transform infrared spectroscopy (FTIR). The results of a study of the gel-sol transition time at a physiological temperature of 37 °C for samples of the design thermo-responsive bioactive gelatin-alginate-humic nanocomposite hydrogel containing 6.4 % wt. of sodium alginate and 14 % wt. of gelatin visually showed a sharp increase in the transition time from 6 min to 11 min as a result of adding 2.5 % wt. of humic acids. Thus, these studies showed that relatively small concentrations of humic acids can provide a prolonged drug delivery effect through the use of gelatin-alginate-humic nanocomposite hydrogel on the surface of the human body.

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# The Antimicrobial Effectiveness of the Hydroxyapatite Matrix Loaded With Metal Nanoparticles

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**Abstract ID #NRA-1049**

Hydroxyapatite (HA) based materials are widely used in dentistry and orthopedy due to the biocompatibility, porosity, osteoinductivity and non-toxicity [1,2]. HA could be combined with other components (ions, polymers, nanomaterials) to provide bone substitutes. However, the use of bone grafts can lead to the infections, caused by the attack and proliferation of bacteria at the site of the application [1,3]. Recent investigations illustrate significant growth of antibiotic-resistant bacteria leading to search of novel antibacterial agents, that could help decrease of the problem of antibiotic resistance. Metal and metal oxide nanoparticles (NPs) could successfully replace antibiotics, showing intrinsic antibacterial activity to the target bacteria [4]. Nanomaterials exhibit toxic effects against several bacterial strains and, due to this, could be successfully used for biomedical applications, including drug delivery and tissue engineering. High dosage of NPs could induce toxicity for eukaryotic cells, besides a low dosage, sublethal for bacteria, increases the permeability of the bacteria cell membranes [4]. To minimize infections related with the use of bone substitutes, composite materials based on hydroxyapatite with addition of AgNPs and CuNPs were synthesized in this work. Their antimicrobial influence for highly virulent and antibiotic resistant bacteria (E. faecium, S. aureus, K. pneumonia, A. baumanii, P. aeruginosa and Enterobacter spp.) were compared. These pathogenic strains belong to the group named ESKAPE [5]. Synthesis of stoichiometric hydroxyapatite was provided by following reaction:

$$10CaCl_2 + 6Na_2HPO_4 + 8NaOH \rightarrow Ca_{10}(PO_4)_6(OH)_2 + 20NaCl + 6H_2O$$

Cu NPs were synthesized by polyol synthesis in etylenglycol media. For investigation of antibacterial properties of AgNPs in composite with hydroxyapatite, commercial suspension of AgNPs NanoPure (Poland) was used. HA was mixed with calculated volume of NPs suspensions for obtaining of required Cu concentrations (250, 500 and 1000 μg/g) and Ag (25, 50, 75, 100 μg/g) in composite. The dried powder was grinded in agate and pressed in tablets with mass 150 mg with diameter 8 mm. Obtained tablets were used for investigation of antibacterial properties of HA-Cu(Ag) composites.

It was revealed that minimum inhibitory concentration of Ag NPs against listed pathogens varied from 2.5 μg/mL to 5 μg/mL. At the same time MIC of Cu NPs nanoparticles was higher and varied from 4 μg/mL to 145.3 μg/mL. Contact inhibition of the strains by composites of HA and Ag NPs and Cu NPs and revealed the effectiveness of both types of nanoparticles. It was found that adding Ag NPs to HA caused more effective antibacterial activity than adding of the Cu NPs to HA.

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# Characteristics of the MXene-Anti-CEACAM1 Complex For Photothermal Targeted Treatment of Melanoma

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**Abstract ID #NRA-1052**

Local photothermal therapy (PTT) represents a promising non-invasive treatment modality. The operating principle of the PTT is based on the presence of optical absorbing agents, also known as photothermal agents (PTAs). The importance of the presence of PTAs is due to their ability to absorb and convert light energy into heat. Thus, tumor cells associated with PTAs are amenable to thermal ablation [1, 2]. In our study, we consider MXenes as PTAs for the photothermal ablation of melanoma [3]. To ensure the attachment of nanoparticles only to tumor cells, we developed an MXene-anti-CEACAM1 complex. Anti-CEACAM1 monoclonal antibody (mAb) exhibits specificity for a CEACAM1 molecule that is expressed on the surface of melanoma cells and can be used as a target for the treatment of melanoma [4]. The combination of MXenes and anti-CEACAM1 mAb emerges as a promising platform for the development of an innovative targeted treatment model for melanoma.

The aim of our study is the development of an MXene-anti-CEACAM1 mAb complex followed by its biological characterization with evaluation of the targeted photothermal effect in vitro using a NIR-I laser.

Delaminated $Ti_3C_2T_x$ MXenes were modified with polydopamine (PDA) with different thicknesses followed by human anti-CEACAM1 mAb immobilization. Biological characterization of the complex included determination of specificity (FACS, ELISA), affinity (FACS, bright field microscopy, $IC_{50}$) and cross-reactivity (FACS).

Results of FACS and ELISA assays demonstrate high affinity and specificity to CEACAM1, while the MXene-PDA-anti-CEACAM1 mAb complex does not bind to other CEACAMs (CC3/CC5/CC6/CC8). Furthermore, increasing the thickness of the PDA layer does not affect the specificity and affinity of the complex.

Conclusion. Our results demonstrate the MXene-PDA-anti-CEACAM1 mAb complex is a promising model for a new model of targeted melanoma PTT. Improvements to this approach, such as surface modification of MXene with PDA and coupling with specific antibodies, could expand its applicability in the treatment of other cancers.

## ACKNOWLEDGMENTS

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# Biocompatibility of modified chitosan films with human erythrocytes and skin fibroblasts (in vitro)

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**Abstract ID #NRA-1061**

Millions of people worldwide suffer acute as well as chronic skin injuries. Wound healing is a complex process due to the involvement of many factors and the complexity of the mechanisms involved. The repair process consists of four main stages: haemostasis, inflammation, proliferation and remodelling [1]. Infection, wound contamination and an extensive area of damage can lead to a delay in the natural skin regeneration process and interfere with the patient's quality of life [2]. In addition, wounds that are difficult to heal and have long recovery times generate high financial costs. For this reason, agents are being sought to accelerate and alleviate the wound healing process. Potential wound healing aids are chitosan films.

Chitosan is a biopolymer obtained by incomplete deacetylation of chitin, which is extracted from crustacean exoskeletons and the cell wall of fungi or bacteria. The most attractive properties from the point of view of wound healing are low toxicity, mucoadhesiveness, haemocompatibility, biodegradability and anti-cancer, antioxidant or antimicrobial properties. The water solubility of chitosan means that it can be used as a colloidal solution from which a hydrogel can be obtained that is responsive to pH changes and formed into films and shaped as self-assembled microspheres [1-3].

The aim of this study was to evaluate the potential of chitosan-based films modified with querecetin and metals (Ag, Au, Cu, Bi) in wound healing by analysing the toxicity of the nanocomposites against human erythrocytes and a skin fibroblast cell line (BJ).

The chitosan films against human erythrocytes had a low toxicity of about 5%, only the nanocomposites combined with silver showed a higher toxicity of more than 10% depending on the amount of silver in the molecule. For cytotoxicity, a similar trend can also be observed, i.e. silver-linked nanocomposites were more toxic than the other chitosan films. The other chitosan films had a good toxicity profile, which provokes further analyses for usefulness in wound healing. The combination of chitosan with other compounds may result in hitherto unknown beneficial characteristics and/or enhance hitherto existing effects, which will improve the quality of life for patients and reduce the value of the financial costs generated.

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# BSA Stabilized Gold Nanoclusters Labelled With Technetium-99m Candidates For Theranostics and Dual Imaging

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**Abstract ID #NRA-1076**

One of the leading causes of death is cancer, thus improvements in early detection and effective treatment is of great importance. Current diagnostic methods might be improved by using new contrast agents and multimodal imaging materials. Optical imaging is a highly sensitive and a high-resolution imaging technique. However, due to low light penetration it is limited to superficial tissue layers. Deep tissue imaging is available by using gamma photons emitting materials, such as technetium-99m ($^{99m}$Tc). However, imaging with gamma photons exhibits lower resolution and requires specific technical requirements. Combining both optical and gamma emitter methods might improve diagnostic capabilities, diagnostics accuracy, and lead to a better patient outcome. One of such dual modality agents might be protein stabilized gold nanoclusters labelled with $^{99m}$Tc (Protein-Au NCs-$^{99m}$Tc). Such an agent would combine fluorescence of gold nanoclusters and gamma photons of $^{99m}$Tc for imaging. We have previously demonstrated that protein stabilized gold nanoclusters can be synthesized using human plasma proteins and are able to generate reactive oxygen species (ROS), therefore, labelling it with $^{99m}$Tc would allow to create a personalized theranostic agent. Such compound may be used for dual mode imaging (optical and gamma) and photodynamic therapy (PDT). In this study a potential of $^{99m}$Tc labelled bovine serum albumin gold nanoclusters (BSA-Au NCs) to generate ROS and be applied as potential theranostic agent in cancer PDT was investigated.

The BSA-Au NCs were synthesized according to the previously reported procedure [1] with slight modifications. To create a multimodal imaging agent the BSA-Au NCs were labelled with $^{99m}$Tc. The standard serum proteins' labelling procedure was used for attaching $^{99m}$Tc to BSA-Au NCs [2]. The binding quality of $^{99m}$Tc to BSA-Au NCs was confirmed by thin layer chromatography. Free pertechnetate ($^{99m}TcO^{4-}$) was migrating on the chromatography strip, whereas, BSA-Au NCs-$^{99m}$Tc complex remained bound at the beginning of the strip. Fluorescent BSA-Au NCs-$^{99m}$Tc signal aligned perfectly with the gamma signal of thin-layer chromatography strips. Fluorescent ROS sensor dihydrorhodamine (DHR) was used for investigation of BSA-Au NCs-$^{99m}$Tc ability to generate ROS under irradiation with 405 nm light (43 mW/cm$^2$). The results showed that this complex generates ROS under 405 nm irradiation (DHR fluorescence intensity increases). Labelling BSA-Au NCs with $^{99m}$Tc had a negative impact on ROS generation efficiency (it decreased by ~ 35%), however, it was almost identical to ROS generation by a conventional photosensitizer Chlorin $e_6$. The ability to generate ROS makes BSA-Au NCs-$^{99m}$Tc a suitable candidate for further investigation as theranostic agent and its' usage in PDT.

The study results showed that BSA-Au NCs labelled with $^{99m}$Tc generates ROS under VIS irradiation and may be used for fluorescence and gamma imaging and is a potential theranostic agent.

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# Delayed Reactive Oxygen Species Production By UV Pre-irradiated Orthovanadate Nanocrystals

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**Abstract ID #NRA-1088**

Reactive oxygen species (ROS) like superoxide anions ($O_2^{\bullet-}$), hydroxyl radicals (•OH), and hydrogen peroxide ($H_2O_2$) are crucial for cellular functions [1]. At low physiological concentrations, ROS act as important redox messengers involved in intracellular signaling and regulation. In contrast, cancer cells maintain ROS levels near the threshold of cell death, making them more susceptible to additional oxidative stress caused by ROS-generating agents. [2]. Over the past decade, research into cancer treatments focused on modulating ROS has expanded significantly. Many researchers have dedicated efforts to exploring diverse strategies for inducing ROS production using various nanomaterials. This approach holds promise for developing effective therapies that exploit ROS to damage cancer cells [3]. That is why, nanomaterials that facilitate the generation of ROS and induce oxidative stress have shown promising potential for various nanomedicine applications.

In this study, we report delayed pro-oxidant activity of UV pre-irradiated orthovanadate nanocrystals in water solutions without any external stimuli (in the darkness). The obtained nanocrystals were characterized using X-ray diffraction, transmission electron microscopy, and X-ray photoelectron spectroscopy. The delayed pro-oxidant activity of the obtained nanocrystals was studied using ROS-specific luminescence probes, as well as by measuring nonspecific dye degradation and lipid autoxidation.

Our experiments have revealed that orthovanadate nanocrystals demonstrate delayed pro-oxidant activity, specifically the generation of ROS, after UV pre-irradiation and subsequently keeping in darkness. This delayed pro-oxidant activity has been linked to the generation of $O_2^{\bullet-}$, •OH, and hydrogen peroxide $H_2O_2$. We hypothesize that the primary source responsible for the effective delayed generation of $O_2^{\bullet-}$ and •OH by orthovanadate nanocrystals in the dark is attributed to the abundance of $V^{4+}$ ions and oxygen vacancies within the crystal lattice of the nanocrystals. Furthermore, due to its unsaturated nature, oxygen vacancy can promote $O_2$ adsorption at the surface of nanocrystals. In dark conditions, this oxygen adsorption can lead to the generation of $O_2^{\bullet-}$ through a reaction involving the electrons stored in $V^{4+}$ ions. Simultaneously, photo-induced holes generated by UV pre-irradiation may become trapped within local metastable levels. These metastable levels arise due to random scattering potentials of oxygen vacancies. The presence of these metastable levels serves to localize the holes, delaying their transfer to the surface of the nanocrystal and generation of •OH.

The delayed redox activity observed in orthovanadate nanocrystals holds great promise for biomedical applications. This distinctive characteristic offers a novel strategy for advancing the treatment of malignant cells, potentially revolutionizing approaches in cancer therapy.

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# Hybrid Borosilicate Aerogels Containing Ca(II) for Bone Regeneration

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**Abstract ID #NRA-1089**

In recent years, bioactive glasses have gathered considerable interest due to their capacity to stimulate the body's natural repair process, known as "osteostimulation"[1,2]. Among the important classes of porous non-crystalline solids is borosilicates, which exhibit rapid decomposition and adsorption rates within the human body [3,4]. To broaden understanding of the relationship between biological activity and structural properties of borosilicate materials, a series of Ca(II)-containing hybrid borosilicate aerogels were systematically designed, synthesized, and examined. Additionally, an extensive structural characterization was conducted, taking into account the influence of Ca(II) sources ($CaCl_2$, $\beta$-$Ca_3(PO_4)_2$, and $Ca_{10}(PO_4)_6(OH)_2$) and biopolymers (PVA (MW: 13000, 49000, 83000), pectin and alginate). A comprehensive characterization method was employed to acquire information on the chemical structure (FT-IR spectroscopy and solid-state NMR), textural properties ($N_2$ sorption and SANS), morphology (TEM and SEM), elemental analysis (EDS), X-ray diffraction, and zeta potential measurements. The potential application of hybrid aerogels in bone regeneration was assessed based on the viability and proliferation of stem cells using the MG-63 osteosarcoma cell line and dental pulp stem cells [5].

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# Improvement of Biosensors Through the Use of Advanced Nanomaterials

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**Abstract ID #NRA-1096**

Immunosensors are analytical instruments that combine the precision of immunological reactions with the high sensitivity of modern sensor technology. Designed to accurately detect specific molecules, usually antigens or antibodies, in various samples such as blood, saliva, or environmental fluids, these instruments play an important role in medical diagnostics, environmental monitoring, and food safety [1]. Surface plasmon resonance (SPR) spectroscopy is a powerful analytical technique used to study biomolecular interactions in real-time. In addition, as a susceptible method, SPR spectroscopy is actively used for the design of various immunosensors [2]. Increasing the sensitivity of SPR immunosensors is possible through the application of nanomaterials. Various nanostructures such as gold nanoparticles, magnetic nanoparticles, MXenes, and Quantum dots can be used for this purpose [3]. The usage of such nanomaterials can reduce the detection limit by more than a hundred times [4].

This research focuses on the use of SPR spectroscopy to create and improve sensitive immunosensors. Using specific examples, it will discuss how nanostructures are used to enhance the analytical capabilities of SPR immunosensors.

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# Analysis of Singlet Oxygen Luminescence Generated By Proyoporphyrin IX For Photodynamic Therapy

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**Abstract ID #NRA-1105**

Photodynamic therapy (PDT) is an emerging cancer therapeutic modality that utilizes light, a photosensitizer, and molecular oxygen to induce localized cell death [1], [2]. Its efficacy is usually mediated by the generation of singlet oxygen ($^1O_2$), a highly reactive excited oxygen species responsible for cell killing. Hence, sensitive monitoring of $^1O_2$ during PDT enables optimal treatment delivery to the tumor target with reduced off-target effects [3]. Its direct observation by measuring its luminescence emission at 1270 nm remains challenging due to the very low signal. Time-resolved Singlet Oxygen Luminescence Detection (TSOLD) has emerged as a powerful technique for real-time detection and quantification of $^1O_2$ during PDT [4], [5], [6]. This study presents $^1O_2$ luminance measurements using an in-house TSOLD system applied to Protoporphyrin IX (PpIX) in ethanol and acetone solutions. The system incorporates a supercontinuum laser, a cuvette containing the photosensitizer solution, custom optical filtering and mirrors, a single-photon avalanche diode (SPAD) detector, and time-tagger electronics. Increasing the concentration of PpIX in these solvents from 1 to 10 mg/Kg resulted in a 3-4x increase in $^1O_2$ luminescence signal. The calculated $^1O_2$ lifetime for PpIX was strongly solvent dependent, being ~14.5 and 48.3 µs in ethanol and acetone, respectively. These results confirm the effect of the biological microenvironment on the singlet oxygen signal and hence on the photodynamic efficacy.

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# Exploring Anaerobic Biodegradation Pathways of Iron Ferrocyanide-based Cellulosic Framework Plastics in Municipal Solid Waste Leachate: Insights and Nanoparticles Strategies

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**Abstract ID #NRA-1132**

The extensive use of polymer materials results in the generation of a significant volume of plastic waste, which is estimated at 300 million tons globally. Approximately 40% of this waste is deposited in municipal solid waste (MSW) landfills, and leachate, a liquid byproduct, is continuously released. Detectable plastic micro- and nano-particles in the leachate poses significant and long-term environmental risks, potentially penetrating physiological barriers, causing irreversible disruptions in human intracellular reproductive, neural, and developmental systems, leading to severe consequences.

This study aimed to elucidate the dynamics of anaerobic biodegradation processes involving iron ferrocyanide and various cellulose-based polymer materials (such as cellulose, cellulose acetate, and nanocellulose) within the leachate of Getlini EKO, Ltd. (Riga, Latvia) MSW Landfill. The investigated substrates were introduced into pressure-resistant glass bottles and incubated at 37°C in the absence of light. Biogas produced during an incubation period of 150 days was collected using graduated syringes. Following biogas release, the finely dispersed digestate was analyzed using X-ray diffraction, Fourier transform spectroscopy, fluorescent microscopy employing Nile Red, and other analytical techniques. A co-polymer containing iron ferrocyanide was synthesized using $Fe(NO_3)_3$ and $FeCl_3$. Iron ferrocyanide nanoparticles were synthesized through thermochemical processes using $K_3[Fe(CN)_6]$ in an acidic medium at varying temperatures (120°C, 160°C, 180°C) and synthesis durations.

Here we demonstrate that the microbial community present in leachate possesses the capability to degrade cellulose or cellulose-based modified materials. Co-polymers containing iron ferrocyanide undergo biodeterioration after an extended initial phase. Nanocellulose fibers exhibit resistance to anaerobic degradation, underscoring the necessity of microbial interactions for the degradation of structured materials. The introduction of iron ferrocyanide nanoparticles and subsequent fermentation under sunlight could promote biodegradation, potentially indicating the photoelectronic properties of iron ferrocyanide nanoparticles that facilitate the aggregation of nanoplastics into larger structures. Insights from this study will be verified in future research.

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# Nanoparticle Delivery in a Human Pancreatic Ductal Adenocarcinoma Organ-On-A-Chip Model

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There is a growing demand for therapies, personalized treatment, and diagnostic approaches for pancreatic ductal adenocarcinoma (PDAC). Protocols to establish human pancreatic organoids have been developed that offer ways to model pancreatic and allow efficient enrichment of patient PDAC cells. These cells can be further introduced in organ-on-a-chip (OOC) systems with or without endothelial barrier. Such OOCs offer constant physiological flow, which is particularly relevant for ductal epithelial structures, and could be used versatile nanoparticle transport and delivery studies.

The aim of this study was to establish PDAC OOC with functional endothelial layer for the assessment of barrier function and nanoparticle transport. For that, primary human PDAC organoids and Human Umbilical Vein Endothelial Cells (HUVEC) were used. Cells were cultured in a vertically stacked design chip made from cyclo-olefin copolymer and a porous PET membrane under varying media flow (1 – 4 ul/min) in cell-specific media. HUVECs were seeded in the bottom channel of the microfluidics chip. After four days of endothelial cell culture, enzymatically digested PDAC organoids were seeded in the upper channel. We used cascade blue and Qdot 655 nanoparticles by applying them in the bottom endothelial channel. Chip outflows from both channels were collected and analysed. OOC without cells were used as controls. We describe the permeability of the endothelial/epithelial barrier under various flow conditions in primary PDAC-OOC with the tested compounds and particles and identify limitations of such approaches.

We have successfully established a PDAC OOC system with endothelial cells that can be maintained in culture on the chip up to several weeks and repeatedly used for, various compound and nanoparticle transport studies under varying flow conditions. Nanoparticles offer a broad application repertoire in theranostics and OOC could serve as platforms to study their transport and delivery.

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# Beyond Immunotherapy: Synergizing Target Modules and Gold Nanoparticles for FAP-Positive Cells Sensitization and Photothermal Applications

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The Fibroblast Activation Protein (FAP) plays a pivotal role, particularly in cancer, being overexpressed in the microenvironment of solid tumors, rendering it an attractive target. Based on the UniCAR platform technology, UniCAR target modules (TMs) have been engineered to specifically address this antigen. These TMs, comprising either a single-chain variable fragment (ScFv) or immunoglobulin G (IgG) format, coupled with the UniCAR peptide epitope E5B9, act as a bridge between universal CAR-T cells and target cells, enhancing safety, and efficiency [1]. This study explores gold nanoparticles (AuNPs), both spherical and branched, as nanocarriers for anti-FAP TMs. Branched AuNPs with NIR absorbance extend beyond conventional targeting, holding potential as photothermal agents for localized therapy. This multifaceted approach aims for enhanced cell labeling, photothermal effects, and cytokine activation, advancing the therapeutic capabilities of anti-FAP-targeted immunotherapy. Surface biofunctionalization of particles was achieved through site-directed immobilization of biomolecule-peptide epitope conjugates, utilizing the cysteine terminus at the peptide epitope, to facilitate the formation of a protein monolayer, allowing precise and stable functionalization. Incubation of the FAP-expressing cell line (HT1080 hFAP) with anti-FAP TM coated NPs, monitored via surface plasmon resonance Scattering (SPRS) imaging, indicated successful cell labeling without inducing toxicity at an optical density of 0.1 OD (~272 pM). Viability assessments conducted on all treated cells demonstrated no toxicity concerns. Specificity testing conducted on PC3 cells, employed as a negative control, revealed no discernible increase in scattering intensity. Ongoing investigations are dedicated to optimizing parameters, including concentration and incubation time, to maximize therapeutic potential, aiming to optimize FAP-targeted nanoparticles for advanced therapeutic and diagnostic applications.

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# Some Aspects of the Development of Nanomaterial-Based Immunosensors

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Researchers continuously explore innovative technological strategies to develop ultra-sensitive, selective, rapid, affordable, and precise immunosensors. With the rapid advancements in nanotechnology, nanomaterial-based optical immunoassays and immunosensors have emerged as effective tools for detecting challenging molecules at nanomolar to attomolar concentrations [1-2]. Among optical immunosensors, surface plasmon resonance (SPR) based immunosensors are very prevalent due to their distinctive ability to sensitively monitor the biomolecule binding events in real-time.

This research will delve into the most critical and highly promising trends and challenges in the applications of nanomaterials, focusing particularly on the utilization of gold nanoparticles and gold-coated magnetic nanoparticles [3]. Special attention will be given to the optimization of antibody surface density highlighting how different antibody immobilization methods, on a planar or nanostructured SPR sensor disk, affect the performance of immunosensors. Various strategies for enhancing the signal of SPR immunosensors using nanoparticles will be discussed [4]. This information holds significant value as it lays a solid foundation for the design of forthcoming ultra-sensitive optical immunoassays and immunosensors.

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# Radiographically Negative Microcalcifications of Human Aorta: Crystal and Chemical Study

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The biomechanical properties of aortic tissue are directly influenced by calcifications [1]. Previous studies have identified three types of biomineralization in the atherosclerotic aorta: radiographically negative microcalcifications (RNMC), microcalcifications, and macrocalcifications [2]. Micro- and macrocalcifications in the human atherosclerotic aorta are also characterized as spheroidal and massive calcifications, respectively [3]. The chemical-crystalline compositions of these calcifications have been extensively studied [4]. However, there is a significant lack of data regarding the smallest, radiographically negative microcalcifications [5]. Early detection of RNMCs could lead to significant advancements in the early diagnosis and prevention of cardiovascular complications associated with atherosclerosis. The morphological and crystal-chemical differences among aortic calcifications suggest distinct mechanisms and conditions for their growth and development. Understanding these differences is crucial for elucidating the regulation of pathological biomineralization, which may provide new approaches to reducing cardiovascular disease morbidity and mortality.

This study aims to investigate the primary morphological and crystal-chemical properties of radiographically negative calcifications in the atherosclerotic aorta. Sixty autopsy cases were examined, including 30 patients with pathological biomineralization in aortic soft tissues (group I) and 30 control patients with aortic atherosclerosis but no biomineral deposits (group II). To confirm the presence of calcium compounds, samples were stained using the von Kossa and alizarin red. Scanning electron microscopy (SEM) was performed using an SEO-SEM Inspect S50-B with a 10 nm resolution, and transmission electron microscopy (TEM) with electron diffraction (ED) was conducted using a PEM-125K microscope (SELMI, Ukraine).

In group I, microscopic calcifications appeared as rounded piles, small powdery particles, or sand grains with spheroidal shapes. Some microcalcifications exhibited star-like, crystalline, or irregular shapes deeply embedded in connective tissue. Elastic and connective tissue fibers were stratified in regions with localized spheroidal microcalcifications. TEM analysis revealed multiple small (up to 2 μm) light and bright microvesicules with discrete localization. SEM and TEM analyses of group II samples did not reveal any signs of biomineral deposition.

X-ray spectral analysis detected varying maturity levels of calcification samples in group I. Radiographically negative microcalcifications, identified by their Ca/P ratio, consisted of amorphous apatite that suggests that RNMCs should be classified separately from microcalcifications.

Complex analysis suggests the importance of radiographically negative microcalcifications in development of aorta atherosclerotic lession and required systematic analysis for understanding their role in disease progression.

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# Morphological and Compositional Analysis of Biomineral Microdeposits in Non-Small Cell Lung Cancer

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Lung cancer is the leading cause of death from malignant neoplasms in both men and women [1]. While calcification is a well-researched pathological process in many tumors and lung diseases, its occurrence in lung cancer remains poorly understood, and the prognostic value and impact of calcification on lung cancer are still unclear [2]. Our previous studies on biomineral formations in ovarian, thyroid, and breast tumors identified the prevalence of hydroxyapatite [3-5] and this research aimed to evaluate the composition and morphology of biomineral microdeposits in non-small cell lung cancer (NSCLC).

A total of 49 histological samples were obtained from NSCLC patients treated at the Sumy Regional Oncology Center between 2013 and 2018. The samples were stained with hematoxylin and eosin to assess pathohistological changes, and the presence of calcium compounds was confirmed using alizarin red and von Kossa staining. Transmission electron microscopy (TEM) with electron diffraction (ED) was performed using a PEM-125K microscope (SELMI, Ukraine) to assess the composition of microdeposits.

Calcification was detected in 4 out of 49 cases: 2 cases in squamous cell carcinoma of the basaloid type and 2 in mucinous adenocarcinoma. In squamous cell carcinoma, pathological biomineralization appeared as coarse polycyclic fragments, blocks, and debris among necrotic detritus surrounded by tumor layers of squamous epithelium. In mucinous adenocarcinoma, specific rounded lamellar calcifications, known as psammoma bodies, were observed.

TEM analysis revealed that NSCLC calcifications possess a crystalline structure with a wide range of crystal sizes (7 to 300 nm), with the most common sizes being 7-14 nm. These particles aggregate into conglomerates, with the largest crystals forming the core. Uniform brightness in the micrographs and point reflections in the electronograms indicate that these particles aggregate based on the predominant orientation of crystallographic planes. The crystals are metastable and highly sensitive to electron beam irradiation. Under an 11 μA electron beam, rapid recrystallization occurs, likely due to slight sample heating. Reducing the beam current to 5 μA slows the recrystallization process. Electronogram analysis showed that the calcifications comprise hydroxyapatite with $Ca_5(PO_4)_3(OH)$ formula.

The obtained data suggest the importance of biomineralization and microdeposits in the development of lung cancer, but future research is required to understand their diagnostic potential and role in disease progression.

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# Locking the SUMO Switch: Inhibiting Rhes and mHTT Interactions Using De Novo Design To Prevent The Spread of Huntington's Disease

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Huntington's disease (HD) is a terrible neurodegenerative disorder, claiming the lives of 2.27 million people annually. It is essential to create therapies and drugs that target the cause of the disease. HD is caused by an increase in the soluble and mutant forms of the huntingtin protein (mHtt). SUMOylation of mHtt by Rhes (ras homolog enriched in striatum) through the E3 ligase domain triggers the solubility of mHTT. The SUMOylation of mHTT by Rhes is essential for its toxicity.

The spread of mHtt through the brain is facilitated by its toxicity and tunneling nanotubes (TNTs). Inhibition of the cysteine 263 residue on Rhes prevents the formation of TNTs and the spread of mHTT. A model of Rhes and mHTT was constructed using constrained docking. Anchor residues in the protein complex were identified using the web server PocketQuery, which was used to construct small-molecule inhibitors using the web server LEA3D. Eight inhibitors were found through PocketQuery and LEA3D, and an inhibitor for cysteine 263 was created. In order to predict the activity of the inhibitors, a QSAR model was constructed using open-access data on E3 ligase inhibitors. Calculations for the pKd and Gibbs free energy yielded a two-tailed P value of 0.0408 for pKd and 0.0409 for Gibbs free energy, indicating that the Rhes-mHTT inhibitors are more efficient than the controls. Blood brain barrier permeability was tested, and five out of the nine inhibitors were predicted as blood brain barrier permeable. Molecular dynamics simulations indicated that the best SUMO E3 ligase inhibitor (ARG260) and the cysteine 263 inhibitor were stable as they had an RMSD of under 2 Angstroms. Retrosynthetic pathways for the inhibitors were also calculated to facilitate wet-lab synthesis using Spaya.AI and IBM RXN, which indicated high confidence, showing non-difficult synthesis. The inhibitors had low toxicity, with an Acute Oral Toxicity Class of 4 for both inhibitors. The created drugs can also be used as a prophylactic therapy to prevent symptom onset. HD is terrible, claiming millions of lives and tearing apart families. In addition, key interacting residues of the Rhes-mHTT complex were discovered to guide further drug discovery. It is essential to create new therapies to target the SUMOylation and spread of mHtt, such as small-molecule therapies, which this research aims to address.

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# Optofluidic Sensors for Enhanced Pharmaceutical Concentration and Purity Analysis

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During live-attenuated influenza virus (LAIV) vaccine production, it is necessary to test products after manufacture to verify the concentration of virus particles . Typically, this is done using biochemical assays such as the fluorescent focus assay (FFA) [1]. FFA is cell culture-based and requires 1-6 days to complete [2]. With 3 days often being the accepted minimum, the significant time required for the analysis makes it impossible to use FFA and similar assays to monitor the vaccine production cycle in real time. As a result, there is currently no feedback on any process parameters during a production cycle, meaning yield is not necessarily optimal. Assays such as the enzyme-linked immunosorbent assay (ELISA) can be completed in under 3 hours [3]; however, given the dilute nature of impure samples, their sensitivity limits pose a challenge to the quantification of LAIV.

Here, we propose using fibre-enhanced fluorescence to provide purification analytics on dilute vaccine samples. The method employs optofluidic hollow-core photonic crystal fibres (HC-PCFs) that guide light by interference effect in a micro-structured cladding, permitting light guidance at the centre of a microfluidic channel [4, 5]. By surface -functionalising the fibres with antibodies, influenza viruses are immobilised onto the fibre surfaces and then fluorescently labelled. The fibre's waveguiding properties are then used to collect and guide the weak fluorescence of dilute samples, with the extended path length enhancing the overall sensitivity compared to that achieved in conventional fluorimetry methods. The HC-PCF geometry also allows for continuous flow, potentially allowing in-line analytics in a pharmaceutical production setting. The low internal volume of 128 nL per centimetre of fibre path length also means very little sample is required for analysis. This makes this method attractive for situations such as drug discovery, where using 10 µL of sample in a typical assay is not feasible. We anticipate that this alternative detection approach could lead to feedback within 3 hours with greater sensitivity than ELISA while only requiring a very low sample volume. This would assist in increasing the yield and quality of products, thereby reducing the cost of accessing vaccination and improving analytics for drug discovery research.

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# Magnetic Mesoporous Bioactive Glass Nanoparticles Co-Doped with Cobalt And Boron for Enhanced Angiogenesis

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Nowadays, bioactive glasses are already sufficiently well described as biomaterials with a wide range of applicability. They have important properties such as osteoconductivity and bonding with soft and hard tissues [1]. Mesoporous bioactive glass nanoparticles have promising use as drug carriers. During their synthesis, it is also possible to incorporate various therapeutic ions into the glass structure, thereby significantly changing their therapeutic potential [2]. Our study focused on the therapeutic ions cobalt and boron for their potential synergistic effect on angiogenic pathways [3]. Angiogenesis is one of the most important processes in wound healing and the treatment of oncological and other diseases, and finally, of course, in the processes of osteogenesis. To make their use more attractive and make it easier to monitor nanoparticle retention, we have prepared a promising composite for strengthening angiogenesis thanks to the already mentioned therapeutic ions and possible monitoring of the nanomaterial after applying a magnetic field in real time. The synthesis and precipitation of superparamagnetic nanoparticles (SPIONs) was performed in the presence of MBGNs, which led to the accumulation of SPIONs on the surface. The magnetic properties were tested using a SQUID device, and the physicochemical and morphological properties were tested using XRD, XPS, FTIR, SEM, and TEM methods. Subsequently, biocompatibility tests such as WST, real-time PCR, or western blot were carried out. At the same time, this testing was aimed at changes in the expression of genes associated with the signaling pathway of angiogenesis, such as vascular endothelial growth factor (VEGF), hypoxia-inducible factor 1 α (HIF-1α) or fibroblast growth factor (FGF).

This research may presents a significant advancement in the field of biomaterials, nanotechnology, and medical science. It offers a versatile method of enhancing angiogenesis using magnetic mesoporous bioactive glass nanoparticles, which have the potential to revolutionize both therapeutic and imaging applications.

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# Testing Antitumor Combinations of Vitamin C and Vitamin K3 In L929 Fibrosarcoma Cells in the Presence of $CeO_2$ Nanoparticles

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Synergistic antitumor effect of vitamin C and vitamin K3 was reported in the number of papers. Furthermore, there are some evidences of antitumor effect of cerium nanoparticles ($CeO_2$ NPs), which enhanced in combination with medicinal compounds (such as doxorubicin). This study evaluated the possibility of obtaining synergistic antitumor effect for vitamin C and vitamin K3 (menadione) as a part of lipophilic $CeO_2$/cholesterol complex, as well as for water-soluble combination of these components with $CeO_2$ NPs.

L929 murine fibrosarcoma cells (~$2x10^4$ cells/ml) were incubated for 48 hours with $CeO_2$ NPs (2 nm, 10 µg/ml), or water-soluble vitamin K3 (20 µmol), or vitamin C (2 mmol), or $CeO_2$ NPs/cholesterol complex (1 : 0.02), or $CeO_2$ NPs/cholesterol/menadione complex (1 : 0.02 : 0.4) in the presence or absence of vitamin C. The effect of the studied compounds and their combinations on cell viability was assessed using the MTT assay.

The inhibitory effect of vitamin C and water-soluble vitamin K3 was 44.3 % and 65.4 %, respectively. The inhibitory effect of the combination of these compounds (71.2 %) exceeded the effects of individual components. The Combination Index (CI) calculated according to the Response Additivity approach [1] is equal to 1.37 indicating relative antagonism (CI >1) of these substances taken in combination, possibly due to their competition for oxygen during oxidation.

However, the most significant inhibitory effect on cell viability was observed for lipophilic complexes of $CeO_2$ NPs with menadione in the presence of vitamin C resulting in 89.3 % effect. For the combination of water-soluble vitamins C and K3 with $CeO_2$ NPs, this indicator was 83.7 %. In addition the CI decreased for both lipophilic (CI =0.797) and water-soluble combinations of these compounds with $CeO_2$ NPs (CI = 0.850). In this case, when calculating CI, we considered the combined action of water-soluble vitamin K3 and vitamin C as the action of a single component related to cytotoxic effect through induction of reactive oxygen species. CI according to the Response Additivity approach indicates the synergism (CI <1) of these substances taken in combination.

Thus, the data indicate the ability of $CeO_2$ nanoparticles to enhance synergistically the antitumor effect of the combination of vitamin K3 and vitamin C.

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# Electrospun Chitosan/PCL-AgNPs Nanofibrous Membranes as Effective System for Purulent Wounds Treatment

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Purulent wounds represent a significant medical challenge, demanding effective and prompt treatment to prevent further complications and infectious issues. In recent years, there has been growing interest in developing new methods and materials to ensure the effective treatment [1]. Notably, the application of nanostructured membranes with antibacterial and regenerative properties has gained significant interest [2, 3]. In this study, we explore the development of an effective system for care of purulent wounds using Chitosan/polylactic asid (Ch/PLC) membranes enriched with silver nanoparticles (AgNPs) [4]. The main objective of this study is to determine the potential impact of Ch/PCL-AgNPs system on infected purulent wounds healing and their susceptibility to infectious complications.

Ch/PCL nanofibrous materials produced using the electrospinning method, loaded with silver nanoparticles (AgNPs) in a concentration of 100 µg/ml were used for wound treatment. A rectangular wound defect with a total area of 1.5 cm² was excised at back of the rats using a sharp scalpel. Subsequently, a gauze swab soaked in a mixture containing 1.0 mL of microorganisms, including S. aureus, E. coli, and P. aeruginosa (each at a concentration of $5 \times 10^9$ CFU/mL), was inserted into the wound. After wound appearance, daily dressing changes were conducted under aseptic conditions. The colony count determination was performed using the streak plate method on different days (1, 3, 5, 7, 9, 11, 14). Histological samples of wounds from rats were taken on days 4, 11, and 21 of the experiment. Throughout this period, the wound defect reduction was monitored daily to assess changes in wound size.

We notice significant effectiveness of Ch/PCL-AgNPs dressing strategy compared to pure Ch/PCL ones. These membranes exhibit high antimicrobial activity starting from 5th day (providing significant antibacterial effect towards S. aureus, E. coli and complete eradication of P. aeruginosa) and promote accelerated wound healing. Tested samples also maintain biocompatibility, without inducing negative reactions or complications in tissues.

Results indicate that the novel Ch/PCL-AgNPs system is effective in promoting antimicrobial activity, accelerating wound healing, and maintaining biocompatibility. This makes it a promising method for treating purulent wounds.

## ACKNOWLEDGMENTS

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# Tumour Chemosensitization to Cisplatin By $CeO_2$ Nanoparticles

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**Abstract ID #NRA-1198**

Development and synthesis of nanomaterials for biomedical applications, such as nanoparticles (NPs) of $CeO_2$, is of growing interest in scientific community. $CeO_2$ NPs in the range of sizes from 6 to 10 nm synthetized for the current work by Shlapa et al. [1] have been shown to be promising to exploit based on in vitro biological activity studies [1, 2]. Here we are focused on the study of biological effects of these particles in vivo, specifically on the study of their possible chemosensitizing properties, since this field of research remains largely unexplored. For this purpose, adult female Wistar rats with a subcutaneously implanted Guerin carcinoma (solid tumour) received chemotherapy with cisplatin (intraperitoneally 1.5 mg per 1 kg of body weight, twice a week over 3 weeks), and 2 h after each injection of cisplatin they received suspension of $CeO_2$ NPs (intraperitoneally 0.2 mg per 1 kg of body weight). In this group of rats, compared with rats that received cisplatin with no $CeO_2$ NPs, there was further inhibition of tumour growth starting from the 15th day post-implantation ($p < 0.05$). Also, from this day post-implantation until the end of experiment, the average tumour size (volume) in the former group of animals did not change, while that in the latter group continued to grow until the 19th day post-implantation (2.2-fold larger than in the former group). Notably, $CeO_2$ NPs are not toxic with respect to the bone marrow. Although cisplatin can predominantly suppress erythropoiesis, $CeO_2$ NPs were shown to be inert with respect to bone marrow cells of rats treated with cisplatin. Bone marrow cell population compositions were similar in both groups of animals. Thus, these results show that $CeO_2$ NPs can be chemosensitizing in cisplatin treatments of tumours with no aggravating impact to the bone marrow. Further investigations are needed to understand the mechanisms underpinning this finding.

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# Unveiling Theranostic Potential: Exosome Camouflage With Cu-Doped Carbon Dots For Glioblastoma Treatment

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Because of their advantageous characteristics, including their small size (2–3 nm), functional groups, and red emission optical properties, chlorophyll-based carbon dots (CDs) are ideal for drug delivery and imaging applications. In addition, CDs demonstrate a robust reaction to photodynamic therapy (PDT), which highlights the considerable potential they hold in the field of nanomedicine research [1]. The results of this study demonstrated that CDs can be loaded into exosomes that are produced from MSCs quite successfully. Furthermore, research has revealed that CDs maintain their therapeutic properties [2]. Additionally, it was observed that CDs delivered via exosomes had a cytotoxic effect on U87 cells, necessitating much lower CD dosages than if CDs were administered separately. The study assessed the underlying processes of U87 cells' response to free CDs-mediated and CD-loaded exosome-mediated photodynamic therapy (PDT) by analyzing the miRNA profiles of both the cancer cells and the exosomes.

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# Enhanced Refractive Index Sensitivity of Linearly Assembled Gold Nanoparticles for Biosensing Applications

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**Abstract ID #NRA-1220**

Gold nanoparticles (AuNPs) attract substantial interest in biosensing applications due to their unique optical properties, such as localized surface plasmon resonance (LSPR). The near field interactions between individual NPs, e.g. in assemblies or arrays, have a significant impact on LSPR signature. Compared to individual particles, ordered arrangements of AuNPs offer collective plasmonic properties which are more susceptible to variations in the local refractive index (RI). Such local changes in RI also occur when biomolecules attach to the surface of AuNPs. Hence, AuNP assemblies could potentially enable the detection of biomolecules of interest with unprecedented accuracy due an enhancement of RI sensitivity. This study presents a comprehensive investigation of the plasmonic spectra of linear periodic assemblies of AuNPs (590 nm periodicity) against individual particles (50 nm diameter) for biosensing applications. Simulations using Finite-Difference Time-Domain (FTDT) method showed that longitudinal coupling along the AuNP lines is more sensitive to RI changes than transversal coupling. This was further investigated experimentally through an exemplary attachment of the biomolecules to the nanoparticle lines. Tumor Necrosis Factor Alpha (TNF-$\alpha$), a pro-inflammatory cytokine which plays a multifaceted role in cancer research, influencing various aspects of tumorigenesis, tumor progression, and therapeutic response was chosen for the bio-functionalization experiments. Wrinkled polydimethylsiloxane (PDMS) templates were used to confine the $cm^2$ large arrays of amine-functionalized AuNPs into lines on glass substrates. RI sensitivity of the AuNP assemblies during various steps of the functionalization were investigated using UV-Vis spectrometry. Promising experimental results demonstrate enhanced RI sensitivity of the linear assemblies, compared to single NPs, offering a new approach towards plasmonic biosensing applications.

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# Synthesis of Polylactic Acid Membranes Loaded With Silver Nanoparticles By Electrospinning Technique

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**Abstract ID #NRA-1223**

Polylactic acid (PLA) is a biodegradable and biocompatible thermoplastic aliphatic material that could stimulate tissue regeneration and drug release in tissue engineering. It is successfully applied to electrospinning of membranes in biomedical field due to its biocompatibility [1]. Selection of non-hazardous solvents for PLA and their optimal ratio is highly important for biomedical applications and membrane formation. The nanofibers formation and spinnability of solution highly depends on considered mixed-solvent system of polymer [1,2]. In this study we varied polymer concentration, and ratio of solvents (acetone (AC), dimethylformamide (DMF) and chloroform (CHL)) in polymer solution to find effect on the fiber diameter and morphology. The appropriate solvent selection depends on the type of polymer should optimize the electrospinning process to produce homogeneous membranes [3]. The mixture of solvents that are nonpolar – CHL (the dielectric constant lower than 5) and polar – AC and DMF (the dielectric constant higher than 20) used to meet the electrical property criteria. PLA is better dissolved in CHL, but addition of a solvents with higher dielectric constant, like AC and DMF created more charges on the jet surface that enhances the stability of the charged jet facilitating the formation of fibers.
At the first stage was solution preparation for electrospinning. Polylactic acid was dissolved step by step in CHL, AC and DMF in following ratios:

sample #1: (5% PLA+10 mL CHL+ 5 mL AC + 5 mL DMF)

sample #2: (5% PLA+10 mL CHL+ 10 mL AC)

sample #3: (5% PLA+10 mL CHL+ 7 mL AC + 3 mL DMF)

sample #4: (5% PLA+10 mL CHL+ 3 mL AC + 7 mL DMF)

sample #5: (10% PLA+10 mL CHL+ 5 mL AC + 5 mL DMF)

The solution of silver nanoparticles with concentration 3 g/L was added dropwise to the polymer-solvents solutions for increasing antibacterial properties of obtained membranes.

The morphology of obtained membranes and fibrils structure were investigated by SEM (SEO-SEM Inspect S50-B) equipped with energy dispersive spectrometer AZtecOne with detector X-MaxN20 (Oxford Instruments plc.) for element analysis. The main factors that influenced on fibers morphology are voltage and the flow rate. Such parameters should be varied for different polymer solutions. It was observed that fibrils diameter was decreased with increase of voltage. The increase of PLA concentration to 10% leads to increasing fiber diameter. It was concluded that by varying of PLA solution concentrations and electrospinning parameters membranes with oriented fibrils and required diameter will be obtained.

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# Composition and Fine Morphology of Uratic Prostate Stones: A Detailed Analysis

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Prostate cancer (PC) is one of the leading causes of cancer-related deaths worldwide. The development and progression of PC are closely linked to chronic inflammation, often associated with intraluminal inclusions known as prostatic stones (PS) [1]. Infrared analysis has revealed that PS primarily (90.7 %) composed of calcium phosphates. Other mineral phases, such as calcium oxalates, struvite, brushite, octocalcium phosphate pentahydrate, citrates, and urates, have also been observed. These phases are unevenly distributed throughout the stone, often forming layered and periodic structures; the core and surface of the stone can be significantly different in phase compositions [2].

To understand the role of different Ca/P phases in PS development, this study investigates the composition and morphology of uratic prostate stones.

Thirty-six prostate stone samples were obtained from patients at Sumy Regional Hospital and Sumy City Hospital between 2010 and 2024. Scanning electron microscopy (SEM) was performed using an SEO-SEM Inspect S50-B with a resolution of 10 nm to confirm the presence of calcium compounds with further X-ray structural (XRD) analysis.

Due to the multiphase nature and inhomogeneity of phase distribution within the stones, traditional macroscopic materials science methods like XRD and infrared analysis have limitations. To detail the structural phase and chemical composition concerning the morphological features of prostate stones, local analysis methods with micron spatial resolution are required. SEM-EDX analysis, which is accessible and widespread, was applied to thin or cross sections of prostate stones for local analysis at selected points/areas, as well as in mapping and line scanning modes.

Among the 36 X-ray structurally analyzed prostatic stones, 6 were urate, and 5 had a notable admixture of oxalates. This proportion of urate stones is significantly higher than reported in previous studies [3, 4]. SEM analysis of a thin section of a typical urate stone sample with low oxalate content revealed a layered structure. Linear EDX scanning across the layers in the radial direction indicated that calcium phosphate phases predominate in dense, narrow layers, while urate phases predominate in loose, wide layers. The identification of the calcium phosphate phase was unexpected, contradicting the X-ray phase analysis results. This finding suggests a more complex internal structure and composition of uratic prostate stones than previously reported. Notably, the presence of oxalates, commonly occurring as $C_2CaO_4 \cdot H_2O$ (whewellite), was confirmed as the most frequent impurity in urate stones.

Further studies will be necessary to explore the diagnostic and prognostic implications of these findings, as well as their potential impact on the treatment and management of prostate cancer associated with prostatic stones.

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# Addressing The Challenge of Peripheral Nerve Injuries with $Ti_3C_2$ MXene Based Electro-conductive Polymer Nerve Guidance Conduits

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**Abstract ID #NRA-1228**

Injuries to peripheral nerves is a significant public health concern exacerbated by the rise in travel frequency and an unfortunate increase in armed conflicts. While diagnosing these injuries is relatively straightforward, their management poses a considerable challenge. The current gold standard surgical technique involves using autografts using a donor nerve graft from the patient's own body to bridge the injury gap. However, this approach results in additional injury at the donor site, underscoring the complexity of managing such injuries. Moreover, the treatment of peripheral nerve injuries has seen little innovation over the past century, highlighting the critical need for alternative approaches that can effectively address these injuries without causing additional harm to the patient.

Nerve guidance conduits are specialized structures designed to facilitate the repair and recovery of damaged nerves. These conduits, constructed from a diverse range of biomaterials, create a supportive environment for nerve regeneration. While tubulisation utilizing materials like silicon tubing provides a basic solution, it falls short of being optimal. The demand for new biomaterials that are biocompatible, biodegradable and supportive is evident, with a particular focus on polymers to meet these criteria.

Given the electrical nature of neuronal signals, it was suggested to utilize electro-conductive conduits to enhance the efficacy of nerve regeneration. This has led to the development of conductive polymer neuronal conduits, representing a cutting-edge approach to neural recovery. Such conduits hold promise in overcoming the challenges with regeneration of neuronal injuries. Nonetheless, a major obstacle arises: most polymers lack conductivity and instead function as dielectrics.

Addressing this challenge, we employ MXenes, a novel family of graphene-like 2D nanomaterials with exceptional properties. MXenes have attracted significant interest across various scientific and technological domains, particularly for their remarkable electro-conductivity surpassing that of graphene. The non-toxic and biocompatible nature of MXenes makes them ideal candidates for designing the next generation of neuronal conduits. Consequently, our project focuses on developing polymer nanofibrous membranes coated with titanium carbide MXene. These membranes are then employed to construct neural guidance conduits to address sciatic nerve injury in rats. While the project is ongoing, we have already observed enhanced functional recovery in the injured paw treated with the MXene-based nerve guidance conduits.

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# Assessment of MXene Quantum Dot Influence on Tumor Microenvironment Through Spatial Transcriptomics

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**Abstract ID #NRA-1230**

Nanomedicine has emerged as a promising avenue for transforming tumor treatment strategies. However, the complex tumor microenvironment (TME) presents significant challenges, housing diverse immune cell populations alongside tumor cells [1,2]. Despite notable progress in nanoparticle-based therapies, comprehending the intricate interactions within the TME remains a formidable task. In our investigation, we utilized spatial transcriptomics to unveil the gene expression landscape and elucidate the effects of nanoparticle exposure on immune cell dynamics within the TME. Employing $Ti_3C_2T_x$ MXene quantum dots (MQDs), we meticulously tracked their distribution in orthotopic breast cancer models. Our observations unveiled distinct responses in tumour and immune cells based on MQD accumulation, revealing a tumour-suppressive phenotype in regions with variable MQD accumulation. Additionally, pathway analysis and cell deconvolution elucidated alterations in B cells and neutrophils induced by MQDs, encompassing recruitment, activation, and neutrophil degranulation aspects. Using spatial transcriptomics, we comprehensively understood the molecular and cellular changes instigated by MQDs within the TME [3]. Future investigations leveraging spatial omics methodologies with a diverse range of nanoparticles hold significant promise in refining nanotherapeutic design for enhanced efficacy.

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# Effect of PEG 400 Nanocrystal Sizes on Thermal and Spectral Properties

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**Abstract ID #NRA-1240**

Recently, the scale effect for the melting process of nanocrystals in pores has been actively investigated. The influence of the size of nanocrystals and the chemical structure of the matrix surface on the temperature and heat of fusion is widely studied. There are much fewer studies of relaxation processes in nanocrystals. The study of relaxation processes in nanocrystals surrounded by a porous matrix provides information about the mechanisms of thermal mobility of nanocrystal molecules and the influence of the matrix on these mechanisms, which can either block a certain type of molecular mobility or unblock a new one. Such studies are useful for the controlled release of drugs from porous systems, the determination of the temperature range of the pharmacological activity of drugs, and the creation of shape-stabilized phase change materials for use in thermal energy accumulators in solar energy storage systems [1-2].

In our study, silica gels with different pore sizes were filled with polyethylene glycol (PEG) PEG 400. PEGs are widely used in cosmetics as emulsifiers, moisturizers and skin conditioners, in pharmacology as solvents and dispersing agents in the production of drugs, and for drug delivery. [1,3].

The samples were studied by thermophysical, dielectric and spectral methods. The temperature dependences of the specific heat capacity and dielectric permittivity were obtained. It is shown that low-temperature dielectric relaxation is observed in PEG 400 in the range from -64 to -20°C, the melting temperature is equal to 6°C. As the size of PEG nanocrystals decreases, the melting point drops. The effect of increasing the dielectric relaxation temperature is observed for PEG nanocrystals in porous matrices. However, the region of dielectric relaxation shifts toward low temperatures with a decrease in the pore size. It is shown that a relaxation process is observed for the dependence of the specific heat capacity in nanocrystals, which is negligible for bulk PEG. It also shifts to lower temperatures as the pore size decreases. Using IR spectra in the temperature range from -170 to 100°C, the mechanisms of thermal motion leading to relaxation processes in PEG were determined. The influence of the scale effect on relaxation processes is analyzed.

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# Exploring the Therapeutic Potential of $T_3C_2$ MXene Using an In-Ovo Model

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**Abstract ID #NRA-1251**

MXenes, a new class of 2D nanomaterials, holds promises for revolutionizing various biomedical treatments. Their unique combination of a large surface area and specific chemical properties makes them ideal candidates for various applications, including biomedicine. In particular, MXenes demonstrated significant potential as photosensitizers, paving the way for a powerful infrared laser photothermal therapy of cancer. However, further exploration is necessary to fully unlock the full therapeutic potential of MXenes.

The in-ovo model is gaining attention as a more ethical and cost-efficient in-vivo alternative to the traditional animal based testing. This approach allows to study the impact of treatments, drugs, or specific conditions directly on developing embryos within a fertilized egg, offering a valuable and economic in-vivo method.

Melanoma, a highly aggressive form of skin cancer, can spread rapidly throughout the body if left undetected. Relatively easy accessibility of melanoma makes it a promising candidate for treatment with photothermal therapy (PTT). This approach is based on the ability of the light of certain wavelengths to penetrate to some extent into the living tissues. Thus, given the superficial nature of melanoma, PTT can be a promising method for targeting of melanoma by low invasive treatment options. Therefore, in this project we aimed at investigating conditions for efficient tumor ablation of melanoma with MXene as the photosensitizer using an in-ovo chicken embryo model.

B16F10 mouse melanoma cells were cultured under standard conditions in a DMEM/F12 medium supplemented with 10% FBS. The cells were loaded with Ti3C2 MXene at 6,25 µg/ml concentration. The fertilized chicken eggs were incubated for 10 days in a standard egg incubator under recommended conditions. Then, a window was created in the egg shell and 2-3 million cells suspended in 50 µl of medium with 5 mg/ml hyaluronic acid were grafted onto the chorioallantoic membrane (CAM). To enhance tumor formation efficiency, the CAM was subjected to a brief, 20-second irritation with filter paper just before cell engraftment. Then, 6-7 days post-inoculation, the eggs were irradiated with a 1064 nm pulsed laser for 80 sec at 3.1 J/cm2 power density, 200 msec pulses at 1 Hz.

The melanoma tumor could be efficiently grown on chicken CAM. The tumor can reach up to 2.5x1.6x1 cm (width x height x thickness) in size and of up to 1.7 grams of weight. The immunohistochemistry analysis confirmed the melanoma nature of the xenograft tumor. Tumors were successfully grown also with the MXene loaded cells. Currently, the experiment is still in progress to figure out possible changes in the structure and dynamics of tumor development after irradiation.

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# Nanodiamonds as Platforms for Improved Drug Delivery

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**Abstract ID #NRA-1256**

Carbon-based nanoparticles have emerged as promising platforms for theranostics due to their small size, chemical inertness, tailorable surface functionalisation and optical properties. Such properties have found great interest in applications such as multifunctional therapeutics and diagnostics for cancer treatment. While carbon-based materials are significant candidates for nanomedicine, nanodiamonds (ND) in particular have attracted increasing attention. Nanodiamonds (NDs) are currently being researched for applications in the biomedical field due to their biocompatibility, tuneable surface chemistry and photoluminescent properties [1]. Their high surface-to-bulk ratio results in a tuneable surface to allow surface conjugation and release of therapeutics.

This work presents investigations on the surface termination-dependant toxicity of nanodiamonds and the application of the chemotherapy drug Fluorouracil (5-FU) via cytotoxic assay using the human leukaemia monocytic (THP-1) cell line. 5-Fluorouracil (5-FU), a cytotoxic chemotherapy treatment, is one of the most frequently prescribed treatments for cancer. However, major drawbacks prevent the full efficacy of the drug at low doses, such as crystalising in solution negatively impacting the cell uptake [2] and requiring a large dose. Work to combat this using metal nanoparticles such as silver has been complicated due to the nature of the drug degrading onto metallic surfaces [3], however, 5-FU has been shown to be stable on diamond surfaces.

Our investigations show nanodiamonds of 5 nm alone do not harm cell viability while increasing 5-FU efficacy. The ND were shown to promote cytokine uptake, increasing the efficiency of the 5-FU uptake [4]. This has been demonstrated in multiple trials where 5-FU has been crafted onto nanodiamonds of positive and negative Zeta-potentials, at different concentrations, with results showing a much lower concentration of 5-FU is needed to reduce cell viability when combined with nanodiamonds.

Consequently, we propose the use of 5 nm nanodiamonds from detonation synthesis, as a platform for improving the therapeutic function of 5-FU. We show a clear improvement of the drug effectiveness when loaded onto ND, increasing the cell death rate while using far less 5-FU. Therefore, the ND/5-FU showed an enhanced permeation of the drug, highlighting the potential of nanodiamonds as biologically safe drug delivery agents with potentially reduced clinical side effects.

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# MXene-Based Photothermal Ablation of Staphylococcus Aureus and Candida Albicans

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**Abstract ID #NRA-1258**

Introduction. Exploitation of photo-thermal abilities of MXenes has shown promising results in the fight against bacterial infections, including antibiotic-resistant strains [1]. MXenes can be activated by near-infrared light (NIR) absorbing laser light and converting it into heat, which can then be used to destroy microorganisms [2]. This light triggers a dual attack: it heats the microbes while simultaneously sharpening the MXene's edges, allowing them to pierce and disrupt the microbial cell membrane. Photothermal technology has the potential to address the challenge of antibiotic resistance and provide more effective treatment options for microbial infections [3].

Aim. Our research focuses on elaboration of the optimal MXene's concentration that delivers the most effective antimicrobial photothermal therapy when combined with appropriate laser irradiation mode.

Materials and methods. To compare the effectiveness of the $Ti_3C_2$ MXene as a photothermal agent (PTA) against different microorganisms (Staphylococcus aureus and Candida albicans at a concentration of $10^5$ colony-forming units per milliliter, CFU/ml), we used MXene suspensions (at concentrations of 0.44 mg/ml and 0.044 mg/ml). Mixtures of microbial suspension and MXene in equal amounts were cultivated for 4 h at 37°C followed by laser exposure for 10 minutes using a setting of 2 W and 10 Hz. The Petri dishes with nutrient media were inoculated with aliquots of the mixture and incubated for 24 hours at 37°C. Evaluation of results was represented in CFU/ml compared to non-treated samples.

Results. MXenes, as PTA, demonstrated remarkable success against C. albicans at both tested concentrations, completely eliminating the fungus. S. aureus was less sensitive to laser exposure, and noticeable microbial growth retardation was observed only at MXene concentration of 0.44 mg/ml. The varying responses of bacteria and fungi to MXene-based photothermal therapy (PTT) can be attributed to differences in its cell wall composition and susceptibility to heat. Moreover, the absence of a significant impact on fungal or bacterial growth in samples treated with MXene alone (without laser exposure) underscores the importance of thermal activation in achieving antimicrobial effects, highlighting the selective nature of MXene-based PTT against different microorganisms.

Conclusion. MXene has the potential to become a groundbreaking weapon against microbial infections. To fully utilize this potential, additional studies are essential to establish a precise protocol for antimicrobial PTT that involves determining factors like the irradiation mode, intensity, and exposure time, taking into account that the cell wall structure and thermal tolerance of bacteria differ from those of fungi, influencing their responses to PTT.

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# Towards Electroconductive Polymer Scaffolds: Polycaprolactone Nanofiber Membranes with $Ti_3C_2$ MXene Surface Coating.

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**Abstract ID #NRA-1263**

Polycaprolactone (PCL) is a biocompatible and biodegradable polymer, widely used in design of scaffolds for regenerative medicine. Versatility of this polymer enables the fabrication of scaffolds with various architecture, porosity and mechanical properties tailored to specific tissue engineering needs. They combine mechanical strength with flexibility, mimicking the natural extracellular matrix of tissues. Such scaffolds are intensively explored in design of e.g. neuronal guidance conduits and cardiac patches. However, given the electrochemical nature of these tissues, it was suggested that their efficient regeneration requires electro-conductive scaffolds. Yet, design of electro-conductive polymer scaffolds is still a challenging task given the dielectric properties of the most used biocompatible and biodegradable polymers, including PCL.

We and others suggested that MXenes, new 2D nanomaterials with intriguing properties, can be used to render the polymer scaffolds electro-conductive. We previously showed that electrospun PCL nanofiber membranes can be turned electro-conductive by a straightforward dip-coating technique. We also suggested a number of procedures to increase hydrophilicity of the PCL nanofibers, e.g. by treatment with oxygen plasma. Here we investigated morphological, electrical and mechanical properties of the electrospun PCL nanofiber membranes coated with 1 to 3 layers of $Ti_3C_2$ MXene after oxygen plasma surface conditioning.

Optical profilometry was performed by confocal microscopy followed by 3D image deconvolution. Measurement of the electro-conductivity was done with the HIOKI IM7585 Impedance Analyzer. The tensile strength was measured using strips of the membranes 3 mm x 20 mm in size with Instron tensile stress system.

We found that the membranes with MXene surface layers had enriched surface topography and higher surface roughness in comparison to the nascent membranes. Pre-conditioning of the surface with oxygen plasma further contributed to enrichment in surface topography and increase in roughness. Increasing the number of MXene layers to 2 and 3 did not lead to further increases in these parameters.

Electrical impedance was the lowest in the case of PCL-2 coat membranes. Moreover, the increase in the number of layers did not lead to further decrease in impedance. Assessment of phase angle suggested that the MXene layers were deposited on both sides of the membrane with few contacts between them.

The tensile strength at the point of tearing off was the highest with 1 coating layer of MXene. Further increase in the number of MXene layers to 2 and 3 led to noticeable decrease in the tensile strength down to values lower than the non-coated membrane. Pre-conditioning of the fibers with oxygen plasma had no effect on the tensile strength of the membranes.

Overall, research in PCL scaffold design hold promise for advancing the field of regenerative medicine.

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# Potential Immunomodulatory Effects of $Nb_2C$ and $Ti_2C_3$ MXenes on Human Macrophages

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**Abstract ID #NRA-1269**

Macrophages are essential components of innate immunity, playing a crucial role in the defence against pathogens and foreign materials. Polarisation of these versatile cells affects modulating inflammation and repair, and also impacts adaptive immunity reactions. MXenes, a class of two-dimensional transition metal carbides, nitrides or carbonitrides, have gained significant attention due to their unique properties and potential applications in various fields, including biomedicine. While the interaction of macrophages with MXenes has not been addressed yet, it can provide insights into the potential immunomodulatory effects of these nanoparticles. Therefore, this study aimed to investigate the interaction of MXenes, specifically $Nb_2C$ and $Ti_2C_3$, with human macrophages in vitro.

For defining macrophage phenotype and activity, expression of CD68, CD163 and COX-2 was assessed after lipopolysaccharide (LPS) and MXene exposure. Peripheral blood mononuclear cells (PBMC) were isolated from human donor blood using density gradient centrifugation and 100,000 cells/cm2 were plated on glass slides in 24x well plates in standard complete cell culture medium. After 10-14 days in culture, part of PBMCs attached and differentiated to ~1000 macrophages/cm2, while the rest of the cells did not adhere and was washed away. Six experimental groups were established: a control untreated group; cells incubated with $Nb_2C$ MXenes for 1 and 3 days; cells incubated with $Ti_2C_3$ MXenes for 1 and 3 days; and cells stimulated with LPS (100 ng/ml) for 24 h. MXenes were used at 25 μg/ml. After incubation, cells were fixed in 4% formaldehyde for 10 min in PBS and subjected to immunocytochemistry analysis.

Morphological analysis revealed that $Nb_2C$ and LPS treated cells appeared larger in size compared to the control group, whereas the size of the $Ti_2C_3$ treated cells did not change. In the $Nb_2C$ MXene group, COX-2 expression was significantly higher compared to the control group, CD68 expression did not differ between groups, while CD163 expression was elevated compared to the control group. The $Ti_2C_3$ MXene group showed no differences in COX-2, CD68, and CD163 expression as compared to the control group. However, the analysis was hindered by the presence of an intensive black background, likely caused by the phagocytosed MXenes, making accurate assessment challenging. In the LPS group, COX-2 expression was higher than the control group, CD68 expression was elevated, and CD163 expression was significantly higher than the control group.

Consequently, this study demonstrated that MXene can modulate macrophage polarisation in vitro. Various types of MXenes differ in their effect on macrophage phenotype, demonstrating specific properties. Further investigations are required to investigate doze-dependent effect and decipher the mechanisms of various MXene influence on macrophage polarization and functional activity.

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# Nanoparticles Enabled Intravenous Sonothrombolysis

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**Abstract ID #NRA-1287**

Venous thrombosis can cause severe complications influencing tens of millions of people per year worldwide. Ultrasound-mediated thrombolysis (sonothrombolysis) presents a promising treatment for venous embolism. In this talk, nanoparticles enabled sonothrombolysis using ultrasound catheters is reported for enhanced treatment of venous thrombosis. In specific, we investigated microbubbles and nanodroplets mediated sonothrombolysis of both retracted and fresh clots, in vitro with bovine blood clots and in-vivo with a swine deep vein thrombosis model, using small aperture piezoelectric ultrasound transducers. We also studied the magneto- sonothrombolysis using microbubbles coated with magnetic nanoparticles, which showed significantly enhanced lysis rate. Moreover, sonothrombolysis was also successfully demonstrated in-vitro with a laser ultrasound transducer consisting carbon nanoparticles embedded in a PDMS matrix. These findings suggest that nanoparticles enabled sonothrombolysis is very effective in dissolution of thrombosis. Perspectives of nanoparticles enabled ultrasound will be discussed at the end of this presentation for advanced ultrasound sensing, imaging, therapy and drug delivery.

# Active Biophotonic Materials via Patterning and Printing

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**Abstract ID #NRA-1288**

Bio-enabled nanomaterials represent a class of functional materials, which uses bio-derived materials, bioinspiration and biomimetic approaches to design functional nanomaterials and structures mimicking bio-inspired entities [1]. Natural polymers, such as polysaccharides and plant-derived nanocelluloses in particular, self-organize into hierarchical structures, enabling mechanical robustness, bright iridescent color and emission, and polarized light reflection important for active photonics, optical filters, photonic coatings, chiral sensors, and optical encryption and electronics. This set of biomimetic functionalities is engendered by high- aspect ratio cellulose nanocrystals and nanofibers, which exhibit a left-handed helical organization. Here, we summarize our recent results on adaptive chiroptical materials with pre-programmed chirality.

Firstly, we demonstrate that weak magnetic fields can be exploited to create complex optical appearance with local gradients alternating the local chirality of one-dimensional needle-like magnetically decorated cellulose nanocrystals [2, 3]. The formation of optically-patterned thin films with left-, right-handed chiral, and achiral regions was caused by local magnetically- driven vortices. We traced the localized flow directions of the magnetically decorated CNCs during evaporation-induced assembly to show that evaporation and magnetic field-induced localized flow vortices in control of the chiral organization.

Secondly, we fabricated optically active films with pre-programmed handedness (left or right) can be constructed via layer-by-layer shear-induced printing with clockwise and counter- clockwise twisted printing vectors [4]. The resulting large-area thin films are transparent yet exhibit pre-determined mirror symmetrical optical activity, enabling distinction of absorbed and emitted circularly polarized light with different twisted organization and inverted on- demand helicity. The resulting films possess complex light polarization behavior due to step- like changes in linear birefringence and give rise to pre-programmed circular birefringence and photoluminescence, not seen in conventional natural films.

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# Understanding the Mechanism of DNA Fragmentation by MXene in DNA Comet Assay through In-vitro Electrophoresis

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**Abstract ID #NRA-1294**

MXenes, a novel family of 2D materials, are considered highly promising for a wide array of application due to their extraordinary properties and structure. Studies have demonstrated their minimal toxicity, excellent biocompatibility and favorable interactions with biological systems. It is becoming increasingly clear that MXenes will soon find their usage in many biomedical applications.

Despite being actively investigated, the genotoxic properties of MXenes are yet to be thoroughly examined. Our previous research employing DNA comet assay unveiled the substantial occurrence of DNA comets in diverse cell cultures following the exposure to $Ti_3C_2$ and $Nb_4C_3$ MXenes. The precise source of the observed DNA fragmentation remains elusive. We hypothesized that the sharp edges of MXenes may instigate DNA breaks when subjected to an electric field during the electrophoresis step in the DNA comet assay.

In order to test this hypothesis, we devised the technique of in-vitro electrophoresis. For this, cells were cultured in 6-well plates and loaded with MXenes. Two platinum electrodes were positioned at opposite sides of the cell culture wells using 3D printed polymer inserts, and an electric field was applied, mirroring the conditions employed in the DNA comet assay. Cell viability was monitored by resazurin reduction assay.

It was anticipated that if the MXenes indeed could fragment cellular chromosomal DNA while moving in the electric field, the MXene loaded cell would undergo apoptosis or necrosis when exposed to the electric field. We found that the electrophoresis conditions indeed compromised cell viability, potentially attributable to pH alterations. However, reliable detection of the increased cell death in the presence of MXenes under electrophoresis conditions could not be consistently achieved. Moreover, we did not observe any effect of MXenes on cell viability when we placed the whole cell culture plate with the MXene loaded cells in a strong electric field.

The outcomes of the in-vitro electrophoresis and the molecular mechanisms of the DNA comets in the presence of MXenes continue to be the subject of ongoing debates. However, it is becoming increasingly clear that the observed DNA fragmentation manifested in the DNA comets were the result of the artefact of the DNA assay which could not be verified in the independent assays. Further studies are required to uncover the mechanisms of the DNA comets, while the nature of MXene genotoxicity, suggested by the DNA comet assay, remains elusive.

. **ACKNOWLEDGMENTS**

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# Copper Nanoparticles in Ch/PLA Dressing Material Promotes Wound Healing

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Recently, the number of patients requiring wound care has increased significantly. This issue is particularly critical in Ukraine, where the incidence of wounds and injuries among civilians and military personnel has surged since the onset of the full-scale Russian invasion. Standard wound care treatments often face the challenge of bacterial antibiotic resistance, highlighting the need for novel therapeutic strategies. Copper nanoparticles (CuNPs) present a promising alternative to antibiotics in wound treatment due to their antibacterial properties and capacity to promote tissue regeneration. This study investigates the effectiveness of chitosan/polylactic acid (Ch/PLA) dressing materials embedded with CuNPs in the healing of skin wounds.

In this study, Ch/PLA materials with CuNPs were applied to treat skin wounds in rats over 21 days. The dressing materials were changed daily under aseptic conditions. Histological evaluations and immunohistochemical staining of skin samples for M1 (CD68) and M2 (CD163) macrophages were conducted on the 3rd, 11th, and 21st days of treatment.

Our findings indicate that Ch/PLA dressings with CuNPs stimulate the recruitment of M1 macrophages during the initial stages of treatment, exhibiting a pro-inflammatory effect. The number of M2 macrophages increased progressively throughout the treatment period, reducing acute inflammation and modulating the immune response via anti-inflammatory pathways.

Ch/PLA-CuNP dressings exhibit multifaceted modulatory actions on the inflammatory response in wound tissue. They promote the involvement of pro-inflammatory M1 macrophages during the early stages of healing (corresponding to the acute inflammatory phase) and enhance the activity of anti-inflammatory M2 macrophages during the later stages of wound healing. In contrast, skin tissue samples from the Ch/PLA control group (without CuNPs) showed significant necrotic changes, substantial connective tissue, fibrosis, and inflammatory infiltration.

Therefore, due to their potent antimicrobial properties and reparative potential, copper nanoparticles effectively eliminate bacteria in wounds. When combined with Ch/PLA dressing materials, copper nanoparticles facilitate tissue repair and expedite wound healing.

## ACKNOWLEDGMENTS

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# MXene Quantum Dots for Cardiac Regeneration And Repair

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**Abstract ID #NRA-1302**

Stem cell therapy has demonstrated potential for cardiac regeneration and repair following a damage due to injury. In fact, allogeneic stem cells including bone marrow derived mesenchymal stem cells (MSC) and induced pluripotent stem cells (iPSC) have shown beneficial effects after transplantation in the heart. However, poor survival of transplanted stem cells in the infarcted heart has impaired the clinical translation of stem cells-based therapies. We found that allogeneic stem cells after transplantation in the ischemic heart turned immunogenic and were subsequently rejected by host immune system. In our ongoing studies we are developing biomaterials-based strategies to prevent rejection of transplanted stem cells in the heart. We synthesized and characterized MXene quantum dots (MQDs). MQDs possess intrinsic immunomodulatory properties and selectively reduce activation of $CD^{4+}IFN^{-\gamma+}$ T-lymphocytes and promote expansion of immunosuppressive $CD^{4+}CD^{25+}FoxP^{3+}$ regulatory T-cells in an activated lymphocyte population. We also incorporated MQDs into a chitosan-based hydrogel to create a 3D platform for stem cell delivery to the heart. This composite immunomodulatory hydrogel-based platform improved survival of stem cells and mitigated allo-immune responses. We also found that MQDs have potential to mitigate allograft vasculopathy and prevent rejection of transplanted organs. These studies highlight the potential of MXene nanomaterials for regenerative medicine.

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# Synthetic Magnetosomes Integrate Chemotherapy And Hyperthermia in Pancreatic Cancer Cell Model

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**Abstract ID #NRA-1303**

This presentation will describe the development of a new type of synthetic magnetosomes (SMS) designed to combine chemotherapy with magnetic fluid hyperthermia (MFH) for therapeutic purposes, specifically targeting PAN02 cells, a well-established model for mouse pancreatic ductal adenocarcinoma. These SMS consist of magnetically responsive, lipid-based nanosystems encapsulating the chemotherapeutic agent cisplatin. We detail the structure and properties of these magnetosomes, highlighting their remarkable Specific Loss Power (SLP) for heating and drug loading capacity. While 'empty' SMS (without cisplatin) exhibit low cytotoxicity, the cisplatin-loaded SMS demonstrate enhanced drug delivery to PAN02 cells. Structurally, the SMS are composed of magnetic nanoparticles (MNPs) coated with a lipid layer, forming curvilinear and spiral structures similar to those produced by magnetotactic bacteria [1] due to intrinsic dipolar interactions and surface interactions from the lipid layer. The heating capabilities of SMS differ from those of MNPs in gelatin-fixed samples, but a significant increase in SLP for MNPs under in vitro conditions results in an SLP of approximately 1600 W/g ($f$ =765 kHz; $H_0$ = 29 kA/m). Notably, SMS internalized by PAN02 cells maintain similar SLP values as in gelatin, while MNPs show a fourfold increase in SLP upon cell incorporation. Furthermore, SMS demonstrate synergistic effects when combining MFH and chemotherapy in vitro from a single dose, proving more efficient than individual treatments of cisplatin or MFH alone, even surpassing their combined effects. We discuss the implications of these synergistic outcomes.

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# Nanoscopic Sensors in the World of Cancer Research

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**Abstract ID #NRA-1304**

Immunotherapy using CAR-T cells is a new paradigm technology for cancer treatment. To avoid severe side effects and tumor escape variants observed for conventional CAR-T cells approach, adaptor CAR technologies are under development, where intermediate target modules redirect immune cells against cancer cells. In this work, silicon nanowire field effect transistors are used to assist in the development of target modules for an optimized CAR-T cell operation. Focusing on a library of seven variants of E5B9 peptide that is used as CAR peptide epitope, we performed multiplexed binding tests in serum using nanosensor chips. Peptides have been immobilized onto the sensor to compare the signals of transistor upon titration with anti-E5B9 antibodies. Correlation analysis of binding affinities and sensitivities enabled a selection of best candidates for the interaction between CAR and target modules. Finally, cytotoxic functionality of CAR-T cells in combination with the selected target modules were successfully proven. Our results open the perspective for the nanobiosensorics to go beyond the early diagnostics in the field of clinical cancer research, and paves the way towards personalization and efficient monitoring of the immunotherapeutic treatment, where the quantitative analysis with the standard techniques is not an option.

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# Unexpected Local Impact of Nanoparticle Application in Vivo: Adipose Tissue Browning

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**Abstract ID #NRA-1312**

Biomaterials play multiple roles in medicine being applied in various fields, including dentistry, orthopedics, surgery, oncology imaging, cardiology, dermatology and cosmetology, regenerative medicine, imaging and laboratory diagnostics, etc. [1]. Interacting actively with host cells and tissues, biomaterials exhibit various effects from cyto- and genotoxicity to modulating fundamental biological processes including cell proliferation, migration, differentiation and death [2,3]. Besides, nanomaterials also demonstrate a wide range of microbicide and bacteriostatic effects, impacting infectious processes, inflammation and tissue regeneration [3, 4, 5]. Metal-containing nanoparticles and biomaterials have been extensively investigated for the development of antimicrobial drugs, modulating the infected wound process. In this report, we aim to demonstrate the unexpected effect of metal-containing nanomaterials application.

The data were obtained during the studies with Ag-nanoparticles, silver nanoarchitectures (AgNAs), as well as Mg-containing biomaterials [3,4,5], conducted in vitro and vivo experiments. The goal of Ag-containing nanomaterial application was to assess the effect on purulent wound healing [5], while another study aimed to evaluate the safety of Magnesium Implants subcutaneous implantation after a specific coating procedure. The results of the studies revealed the positive impact of Ag-containing nanoparticles and AgNAs on wound clearance and healing. Additionally, we observed unexpected effects related to the transformation of hypodermis from white toward brown adipose tissue. Interestingly the same effect was observed during coated magnesium implant assessment.

The browning of adipose tissue was found near the zone of biomaterial application and was associated with active angiogenesis with multiple small vessels appearing. This phenomenon possessed the transformation of white adipose tissue to multiloculated brown adipose tissue. This effect was associated with abundant M2 macrophages, aSMA-positive myofibroblasts, and capillary density. Such an effect uncovers new directions of metal-containing biomaterials application, as adipose tissue browning is associated with thermogenesis, lipolysis, and secretion of multiple biologically active substances affecting metabolism and inflammation.

In conclusion, application of Ag-and Mg-containing biomaterials was associated with the unexpected effect of adipose tissue browning, accompanied by macrophage polarization and empowering tissue regeneration potential. Such effect of opens the new directions of biomaterial application for cell and tissue-specific reprogramming in metabolic disorders, including obesity and type II diabetes, and regenerative medicine.

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# Modeling of Nanomaterials for Empowering Radiofrequency and Microwave Hyperthermia Treatment

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**Abstract ID #NRA-1313**

The use of electromagnetic (EM) fields in biomedical applications is becoming increasingly popular due to their potential to enhance treatments for cancer and inflammatory diseases, as well as to improve diagnostics and monitoring [1]. Current clinical treatments have notable limitations: (i) surgery is invasive, (ii) radiotherapy requires specialized facilities, and (iii) systemic chemotherapy has significant side effects [1]. Thus, alternative therapeutic approaches are needed. EM fields, particularly radiofrequency (RF – ranging from a few Hz to hundreds of kHz) and microwave (MW, from 300 MHz to 300 GHz) signals, have been investigated for their ability to remotely induce cell apoptosis or necrosis through hyperthermia (HT). Hyperthermia involves heating a targeted area to 40-43°C for at least 60 minutes, creating a cytotoxic environment for diseased cells by altering pH, inducing oxidative stress, and affecting protein folding [1].

Various clinical strategies exist for administering hyperthermia treatment, such as applying a time-varying electromagnetic field to a specific body region, which dissipates heat in biological tissues. This method can be enhanced with nanoparticles, which can improve heat delivery and targeting. Clinically, antenna arrays are often used to generate MW fields to heat targeted neoplastic tissues. The temperature increase resulting from EM field exposure can be analyzed using Pennes' Bio-Heat equation (PBHE) [1].

Despite its potential to control recurrence rates, a major limitation of MW HT is its specificity and selectivity in EM heating. Advances in nanotechnology play a crucial role in improving EM-based techniques for both treatment and detection. Nanosystems can be tailored in terms of size, shape, and composition to respond to electromagnetic fields. Additionally, nanoparticles can be engineered to selectively target lesions, enhancing the localization and effects of EM fields on tissues, thus achieving effective hyperthermia treatment [1].

However, there is currently a gap in applying an electromagnetic engineering perspective to the design and use of nanomaterials as EM-responsive systems as hyperthermia agents for cancer treatment. This work will analyze and discuss recent methods for modeling RF- and MW-responsive nanomaterials for hyperthermia. In particular, it will be discuss how to model the RF and MW response of nanosystems in tumor and biomaterials, , focusing on the heat dissipation. Furthermore, the attention will be brough to the need of accurate and specific multiphysics models. Finally, future perspectives will be offered to bridge the gap between nanomaterials science and electromagnetic engineering.

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# DNA Nanostructures for Antimicrobial Therapy

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**Abstract ID #NRA-1314**

DNA origami [1], i.e., the folding of a long, single-stranded DNA scaffold into an arbitrary 2D or 3D nanoscale shape upon hybridization with a large set of short synthetic oligonucleotides called staple strands, has become a widely employed method for synthesizing fully biocompatible, biodegradable, and nontoxic nanocarriers for biomedicine [2]. Most intriguingly, the DNA origami nanostructures can be modified in a precisely controlled manner with sub-nanometer precision to present different functional entities such as proteins, drugs, and recognition elements [3]. Such DNA origami nanocarriers have been investigated extensively for applications in cancer therapy, whereas potential applications in the treatment and prevention of infectious diseases have only recently become a focus of attention [2,4].

This presentation will summarize our recent and ongoing activities directed at synthesizing, characterizing, and testing antimicrobial DNA origami nanostructures for combating drug-resistant bacteria. In particular, we investigate applications of DNA origami nanostructures as nanocarriers in antimicrobial photodynamic therapy and as templates for the synthesis of multivalent antibiotics nanoarrays with enhanced antimicrobial activity. Both approaches are tested against model bacteria and the most promising formulations and approaches are identified.

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# MXene-Polydopamine-Antibody Complex As A Photosensitizer For Targeted Melanoma Cell Ablation

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**Abstract ID #NRA-1322**

Photothermal therapy (PTT) is an innovative method for eradicating tumor tissues by converting light energy into heat using photothermal materials (photosensitizers). When tissue temperatures reach 41°C, a heat-shock response is triggered, altering gene expression and producing heat-shock proteins. An increase in temperature above 42 °C leads to microthrombosis, ischemia, and tissue necrosis, which is in direct contact with the photosensitizer. An essential advantage of this method is the ability to have a contact-free effect on the target area of swollen tissue without contact [1]. PPT agents can absorb rays from ultraviolet to infrared activated by various light sources. However, the most clinically significant is absorption within I (NIR-I 700-950 nm) and II (NIR-II 1000-1700 nm) near-infrared biological windows, which allows to penetrate the tissue to the maximum depth. Many organic and inorganic photosensitizers are known today [2]. Despite promising results, they face challenges such as low biocompatibility, limited tissue penetration, and instability. $Ti_3C_2T_x$ MXene nanosheets modified by polydopamine in combination with targeted antibodies are one of the most promising nanomaterials for PPT [3].

The aim of our study was to assess the target efficiency of the MXene-polydopamine-antibody complex by PTT melanoma cells in vitro using the NIR-I laser.

Testing various irradiation modes (2 W-10 Hz-5', 2 W-10 Hz-10', 4 W-50 Hz-10') on cells showed minimal heating of water, with temperature increases ranging from 4.5°C for 2 W-10 Hz-5' to 13.6°C for 4 W-50 Hz-10'. Concentrations of 50, 25, and 6.25 μg/mL of $Ti_3C_2T_x$ were selected for testing under the 2 W-10 Hz-5' irradiation mode. The results indicated a direct correlation between temperature and Ti3C2Tx concentration. At 50 μg/mL, the temperature reached 47.8°C, significantly higher ($p < 0.05$) than both the 6.25 μg/mL concentration and the control group (0 μg/mL). The 25 μg/mL concentration did not show a significant difference compared to other tested concentrations, except the control ($p > 0.05$). Using specific antibodies on the surface of MXene allowed for effective selective ablation of melanoma cells, minimizing negative effects.

Conclusion. These results showcase the potential of MXene- polydopamine-antibody complexes in cancer PPT. They emphasize the importance of targeted therapies in oncology, presenting a promising approach for the precise and safe treatment of melanoma.

## ACKNOWLEDGMENTS

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# Defining Extinction Peaks of Various Types of MXenes For Photothermal Therapy And Other Biomedical Applications

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**Abstract ID #NRA-1344**

MXenes is a novel class of two-dimensional materials, which have gained significant popularity across various applications [1]. Among their diverse involvements, MXenes have found increasingly extensive use in the biomedical fields. One promising avenue is photothermal therapy, where MXenes can serve as efficient light-to-heat energy transfer photosensitizers. For instance, we showed that $Ti_3C_2$ MXene was suitable for development of advanced photothermal (PTT) protocols with a pulsed 1064 nm near-infrared laser [2]. However, to achieve an optimal energy transfer, it is crucial to identify the wavelength absorbance peak that maximises energy transfer efficiency. Here, we present the extinction spectra of various types of MXenes along with their defined absorbance peaks.

Our experimental setup involved a wide-spectrum 360 - 2600 nm stabilized tungsten-halogen light source (Thorlabs, SLS201L) and an spectrometer (AvaSpec 2048) which were connected though the optical fiber system to the 3D printed cuvette holder with a cuvette inside filled with a tested solution. Specifically, we investigated $Ni_2C$, $Ni_4C_3$, $Ti_3C_2$ and $V_2C$ MXenes.

After acquiring the extinction spectra for each MXene, we calculated the mean absorbance for various concentrations and built the trendline of the extinction. Next, we extracted the extinction peaks by providing a derivative analysis of the trendline (dExtinction/dWavelength = 0).

Our results demonstrate the optimal wavelength values for PTT for each MXene used. For $Ti_3C_4$ MXene, the most used in biomedical research, we observed two extinction peaks at 389 and 765 nm. For $Ni_2C$, the highest peak was at 390 nm, for $Nb_4C_3$ at 420 nm and for $V_2C$ at 380 nm. This data shows that extinction peaks of the most frequently used MXenes lie in the UV region and near it. According to this data, the wavelengths specific for each type of MXenes should be used to reach the maximum efficiency of the photothermal therapy. Moreover, other types of light sources, in combination with the specific MXenes types, could be employed to achieve maximum efficiency in energy transfer, hence photothermal therapy.

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# Machine Learning-Guided Production of a Self-Nanoemulsifying System for Delivery of Anacardic Acid

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**Abstract ID #NRA-1347**

Bioactive molecules from plants remain an important source of drug candidates [1]. However, these have poor in vivo performance due to low water solubility leading to inadequate distribution [2,3,4], which can be counteracted by oil-in-water nanoemulsion drug delivery systems [5]. A limitation preventing the widespread adoption of nanoemulsions is the expensive, time-consuming iterative development process. In this study, we developed a nanoemulsion design by machine learning (ML). We retrieved average particle size and polydispersity index (PDI) data associated to nanoemulsion composition to construct a dataset from literature. A predictive ML model was used to identify improved self-nanoemulsifying systems including olive oil as base and combinations of Tween 20, Tween 80, glycerol, and soy lecithin. The predictive power of the model was determined by DLS. The nanoemulsions were loaded with an organic extract from Amphipterygiym adstringens (a plant native to Mexico) containing anacardic acid. Encapsulation efficiency (EE%) was measured by HPLC, and the cytotoxic activity was evaluated on HEPG2, a human hepatic cancer cell line, and HEK-293, a normal-like human embryonic kidney cell line. The model's accuracy was 81%. The best-performing formulation was 10% olive oil, 60% Tween 20, and 30% glycerol, exhibiting average particle size of 162.8±26 nm, a PDI of 0.234±0.03, and full EE%. The naked nanoemulsion presented no toxicity in HEK-293 but exerted an inhibitory effect on HEPG2 (IC50 20±1.07 mM). Moreover, loading the plant extract into the nanoemulsion increased the cytotoxic effect on HEPG2 in comparison to the naked nanoemulsion, the extract, and pure anacardic acid, yielding an IC50 value of 5.9±1.2 mM. These results suggest that the formulation identified by the model was a successful carrier of the plant extract. This study presents a proof of concept on how ML can reduce the development pipeline of nanoemulsified drug delivery systems.

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# MXene Biocompatibility Depending on Flake Size and Oxidation State

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**Abstract ID #NRA-1349**

Over the last decade and a half, there has been a marked increase in the study of two-dimensional (2D) materials due to their exceptional physicochemical properties. Transition metal carbides, nitrides, and carbonitrides, collectively known as MXenes, were introduced at Drexel University in 2011 by Yury Gogotsi and Michel Barsoum. This emerging group of 2D materials has shown considerable promise in a variety of applications, including lithium and sodium-ion batteries, electrocatalysis, optoelectronic devices, flexible electronics, and healthcare sectors such as cancer treatment, bacteriology, immunology, targeted drug delivery, and tissue engineering. Research into the use of MXenes in biological and medical contexts is crucial for enhancing our knowledge and utilization of innovative materials in health and biotechnological advancements. Investigating biocompatibility and cellular response is crucial for the application of materials in medicine. Despite numerous publications and the established biocompatibility of MXenes, conflicting information regarding their safety persists. The primary reason for the contradictory data on MXene toxicity is the lack of control over their structural and chemical characteristics during biomedical research. Key factors such as flake size, chemical termination, and oxidation states can significantly influence MXene biocompatibility. Considering these aspects, we conducted a comprehensive study on MXene biocompatibility, focusing on their structural and chemical parameters.

$Ti_3C_2$, $Ti_3(CN)_2$, $V_2C$, and $Nb_2C$ MXenes with controlled size, oxidation state, and chemical terminations were provided by Carbone-Ukraine. In this study, we assessed the biocompatibility and cellular response of these MXenes. We utilized the resazurin reduction metabolic assay, flow cytometry with Annexin V/PI for biocompatibility evaluation, BRDU-ELISA assay for proliferation analysis, and ROS generation measurement with 2',7'-dichlorofluorescin diacetate (DCFDA). Human Immortalized Keratinocytes (HaCaT) and Human Melanoma cells (MaMel8bIV) were used in the experiments.

Our data demonstrated that all types of MXenes exhibited high biocompatibility with dose-dependent effects. $Ti_3C_2$ and $V_2C$ MXenes at concentrations above 50 µg/ml showed moderate toxicity, indicating they can be used in biomedical research with certain limitations. The size of MXene flakes can significantly increase toxicity and impact cell metabolism, including extensive ROS generation. Additionally, oxidized materials can affect cell growth and proliferation, which must be considered during their applications.

Overall, our data demonstrate that controlling the size, chemical terminations, and oxidation state of MXenes is crucial for their safe application in biomedical research

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# Biomedical Application of Free-Standing $Ti_3C_2T_X$ MXene Films

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**Abstract ID #NRA-1357**

A new 2D material, MXene, appeared on the research scene recently and has generated considerable interest among scientists from engineers and physicists to biologists and physicians. Among these materials, $Ti_3C_2T_x$ MXene has garnered significant attention due to its unique properties, including high electrical conductivity, excellent mechanical strength, and biocompatibility. Free-standing $Ti_3C_2T_x$ MXene films, in particular, have shown great potential in various biomedical applications, biosensors, biological imaging, and therapeutic diagnosis. The question of how free-standing MXene film interacts with biological systems is becoming increasingly important due to the new nanomaterial's extensive application in biomedical advancements. The aim of our research was to evaluate the biological and structural properties of $Ti_3C_2T_x$ MXene film.

Free-standing $Ti_3C_2T_x$ MXene-film was prepared by Materials Research Center (Kyiv, Ukraine). The surface morphology of MXene film was characterized by scanning electron microscopy (SEM, Phenom ProX, Phenom-World BV, the Netherlands). Static and dynamic contact angles MXene-films were used to evaluate the hydrophobicity/hydrophilicity of a solid surface by video-based optical contact angle measuring equipment OCA 15 EC, Series GM-10-473 V-5.0 (Data Physics, Filderstadt, Germany). Cytotoxicity and proliferation effects of the material were evaluated using human keratinocytes (HaCaT).

Our results demonstrate that the free-standing MXene film has a multilayer composite structure with a rough, disordered surface. Biological investigations have shown that the film is non-toxic, promotes cell proliferation and provides a significant active surface for interaction with keratinocytes. We noticed that after 6 days of incubation in a cell culture medium, the film lost its flexibility and original shape.

To summarize, the free-standing MXene films in combination with polymer scaffolds have a promising future in biomedical applications.

**ACKNOWLEDGMENTS**

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# Bio-derived Cellulosic Nanomaterials: Advancing Hybrid Soft Materials for Nanobiotechnology

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**Abstract ID #NRA-1359**

Nanotechnology advancements have produced a wide array of hard and soft nanomaterials, each varying in shape, size, and composition. Their distinct physicochemical properties hold great potential for advancing multiple fields. Recently, "green" nanoscale materials produced from cellulose, namely nanocellulose, has attracted considerable interest from researchers in biological engineering, biomedical engineering, and materials science. The unique biophysicochemical properties of nanocellulose have driven substantial research efforts, both fundamental and applied, to develop new biomaterials with advanced features. Despite the progress made, there is still ample scope for enhancement and many unexplored opportunities for innovative approaches. This lecture will delve into the latest advancements in designing and fabricating nanocellulose-based bio-hybrid nanocomposites, focusing on their applications in biological engineering and bio/nano medicine. Additionally, it will discuss the current challenges and limitations in nanocellulose technology and suggest potential strategies to unlock the full potential of multifunctional "green" soft nanomaterials derived from nanocellulose.

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# An Alternative Immune Cell Labeling System Based on the New TwoDimensional Nanomaterials MXenes

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**Abstract ID #NRA-1360**

Deepening our understanding of immune cell behavior is vital for creating safe, effective treatments, particularly as immune cell therapy, also known as cellular immunotherapy or cell-based immunotherapy, represents a groundbreaking approach in the treatment of various diseases, including cancer. Transition metal carbides and nitrides (MXenes)1, a novel family of 2D nanomaterials, show promise as advanced trackers for immune cells key for precise diagnostics and therapies. Traditional cell labeling methods have stagnated due to limited chemical options, impeding progress in applied medicine. Moreover, these methods are incompatible with single-cell mass cytometry by time-of-flight (CyTOF), a globally adopted technology that improves classical flow cytometry. We propose an innovative solution utilizing MXenes to overcome these challenges. Our method, Label-free sINgle-cell tracKing of 2D matErials by mass cytometry (LINKED), leverages a novel, biocompatible, multiplexed, label-free detection approach via CyTOF and Mass Ion Beam Imaging by Time-of-Flight (MIBI-TOF)2. This technique overcomes chemical limitations and integrates seamlessly with CyTOF, allowing nanomaterial detection and simultaneous measurement of diverse immune cell and tissue features2. Our work promises to advance immunological research significantly, offering refined cell labeling and tracking techniques crucial for the advancement of translational medicine.

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# High-Dimensional Approaches for Immune Profiling of 2D Materials

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**Abstract ID #NRA-1361**

We recently depicted the "Nano-immunity-by-design" where the characterization of 2D materials is not solely based on their physical-chemical parameters but also on their immune profiling. [1] The immune profiling can be revealed on its complexity by unique, informative ways: high-dimensional approaches. [2,3] We exploited high-dimensional approaches, such as single-cell mass cytometry and imaging mass cytometry on graphene and other novel two-dimensional materials, such as transition metal carbides/carbonitrides (MXenes). [4-6] We revealed that the amino-functionalization of graphene oxide increased its immunocompatibility. [4] Moreover, we combined graphene with AgInS2 nanocrystals, enabling its detection by single-cell mass cytometry on a large variety of primary immune cells. [5] Recently, we reported the immune modulation of specific MXenes, and their label-free detection by single-cell mass cytometry and other high-dimensional approaches. [6-7] Together with our published works, I will present unpublished results on a wider variety of novel 2D materials, Mxenes, MoS2, WS2, and bismuthene. Our results conceptualize that chemical and immunological designs of 2D materials offer new strategies for their safe exploitation in biomedicine.

**ACKNOWLEDGMENTS**

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TRACK 13

# “ULTRASHORT LASER-MATTER INTERACTIONS & MATERIALS PROCESSING”

# Interactions of MXene with Electromagnetic Waves

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**Abstract ID #ULI-1002**

MXenes, which are an expanding family of two-dimensional transition metal carbides and nitrides, show their versatility for electronic and optoelectronic devices working in diverse electromagnetic environments [1]. Their unique set of characters, such as tunable surface chemistry, anisotropic electronic conducting, and atom-scale layers, endows MXenes various electromagnetic functions across the broad electromagnetic spectrum. In particular, MXenes offer chemically controlled optical and electronic properties that facilitate new ways of influencing material interactions with electromagnetic waves over UV-vis, infrared, terahertz, and gigahertz ranges. Combining these features with ease in processing and excellent mechanical properties, MXenes have already shown great promise in electromagnetic applications such as electromagnetic interference shielding, photothermal conversion, thermal management, infrared identification, and wireless communication. Here we show the fundamental interactions of MXenes with electromagnetic waves across the electromagnetic spectrum covering visible light, infrared, and radio frequency [2-5]. We designed electrochemically driven MXene thin films with unprecedented tunable electromagnetic wave absorption and reflection. The representative electromagnetic functional applications will be discussed. Our method is versatile and can facilitate new ways of influencing material interactions with electromagnetic waves over visible, IR, THz, and GHz wavelength ranges, enabling many technical advances.

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# Synthesis and Characterization of Tungsten (W)-Based Nanofluids via Laser Ablation: Insights into Thermal Conductivity

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**Abstract ID #ULI-1045**

In response to the burgeoning demand of our ICT-driven society, there is a critical need for more efficient cooling solutions in nanoelectronics to effectively manage the heat generated by rapidly expanding data storage centers and solar energy technologies. Nanofluids have emerged as a promising solution to meet these cooling demands. This study explores the impact of the molecular polarity of the host fluid and laser parameters on the stability of W-DW (Distilled Water), W-Ethanol, and W-Ethylene Glycol-based nanofluids, which were synthesized using Pulsed Laser Liquid-Solid Interaction. Comprehensive investigations into their optical, morphological, and crystallographic properties were conducted to assess their stability and thermal conductivity. The findings contribute to a deeper understanding of the role of molecular characteristics in enhancing the performance of nanofluids, positioning them as a viable technological response to the heat management challenges in advanced electronic systems.

# Femtosecond Laser Structuring and Associated Optical Phenomena: the Case of Silicon

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**Abstract ID #ULI-1234**

Laser structuring of materials becomes an environmentally friendly alternative to mechanical processing due to less waste, the absence of toxic chemicals, and also allows creating more accurate and diverse structures.

In this research, we study the features of the laser texturing of polished silicon wafers achieved by the irradiation of Ti:sapphire femtosecond laser radiation with different wavelengths (central wavelength of 800 nm, as well as second and third laser harmonics).

The morphology of resultant femtosecond laser-induced periodic surface structures (LIPSSs) depend on many laser parameters, such as the laser beam wavelength, polarization, pulse irradiation energy density, number of the laser pulses, scan speed [1, 2]. The set of laser parameters determines the characteristics of the treated surface.

Laser structuring can be accompanied by a number of associated optical phenomena. In case of silicon, we investigated the surface plasmon (SP) enhanced second harmonic generation (SHG) and optical emission of ablated Si atoms and formed in plasma SiN molecules [3].

The character of the optical emission can be used to diagnosis LIPSS formation. In particular, the ratio of the intensities of the SHG and the atomic Si emission line has been shown to correlate with the diffraction efficiency of the formed surface ripples, thus the ratio has been suggested as a quantitative measure of LIPSS formation in real time [4].

Our results reveal the potential of LIPSS applications using surface enhanced optical phenomena (SERS [1], SP enhanced SHG [3]) on crystalline silicone.

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# GHz Burst Mode Femtosecond Laser Processing

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**Abstract ID #ULI-1246**

Femtosecond laser pulses with GHz burst mode, which consists of a series of femtosecond laser pulse (intra-pulse) trains with a pulse interval of several hundred ps is expected to achieve high-efficiency and high-quality materials processing that cannot be performed by the conventional irradiation scheme of femtosecond laser pulses (single-pulse mode) [1-3]. In fact, we have so far investigated that GHz burst mode shows distinct characteristics in fabrication efficiency, speed, and quality in ablation of copper and silicon, because the laser energy can be deposited onto the target material in a more temporally controlled manner [2, 3]. Specifically, volume, corresponding to ablation efficiency, ablated by the GHz burst mode is significantly higher than that by the single-pulse mode at the same total input energy, and the efficiency increases as the number of intra-pulses increase. Additionally, compared to the single-pulse mode, the GHz burst mode with the intra-pulse number of 20 achieves 23 times higher ablation speed without deterioration of ablation quality, because air ionization can be suppressed due to lower intra-pulse energy even at larger burst pulse energy.

We have further applied the GHz burst mode to form laser induced periodic surface structures (LIPSS) on silicon and titanium and found that the GHz burst mode can create unique two-dimensional (2D) LIPSS [4, 5]. We speculated that hot spots with highly enhanced electric field of incident laser generated in nanogrooves of 1D LIPSS is attributed to the formation of 2D LIPSS by the GHz burst mode. We have also utilized the GHz burst mode for two-photon polymerization (TPP), showing improvement of fabrication resolution as compared with TPP by the single pulse mode.

The GHz burst mode may offer a new possibility for processing other than ablation, LIPSS formation, and TPP. Thus, we believe that GHz burst mode will open new paths to femtosecond laser processing.

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# Femtosecond Laser-Induced Surface Modification: Theory And Applications

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**Abstract ID #ULI-1325**

Laser-induced self-organized structures, known as LIPSS, grooves, spikes et al. represent a universal phenomenon where high-intensity laser beams interact with various materials, giving rise to periodic surface patterns far from diffraction limit. These self-organized structures, characterized by periodic nano-microstructures, emerge spontaneously and have significant attention due to their wide-ranging applications. Usually, LIPSS imprinting on material surfaces is performed by laser pulses with relatively low laser fluences, near or only slightly above the ablation threshold. This requires dozens or even hundreds of laser pulses coupled to the same irradiation spot on the surface to produce the periodic surface relief. It was believed that an increase of the laser fluence well above the ablation threshold would result in disordering or even complete erasure of the periodic structures by the recoil pressure of the ablation plume. Recently an alternative, more advanced method for the fabrication of nanostructures was proposed [2]. This method is based on the use of femtosecond lasers as a single-step process that can lead to the formation of high-quality nanostructures. This study focuses into the formation mechanisms and the diverse practical uses of self-organised nano-microstructures [3,4].

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# Scattering of 3D He-Ne Laser Radiation By Periodic and Random Structures Formed By Femtosecond and Nanosecond Laser Modification of the Surface of Stainless Steel

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**Abstract ID #ULI-1343**

Laser technologies are widely used in mechanical engineering for processes such as laser cutting, laser welding, and heat treatment. These applications employ powerful lasers with continuous emission or lasers operating in millisecond and microsecond time ranges. However, the current focus of researchers is on developing material processing technologies using short-pulse lasers, specifically nano-, pico-, and femtosecond lasers. These lasers are distinguished by their ability to modify material surfaces, creating unique micro- and nanostructures through both thermal and non-thermal mechanisms. Particularly important is the creation of surfaces with periodic structures, which are highly promising for altering surface roughness parameters to improve antimicrobial, hydrophobic, anti-icing, and tribological properties of products. In this context, austenitic stainless steels, including AISI 321, hold a special place in mechanical engineering due to their widespread use in manufacturing a wide range of equipment operating under extreme conditions, requiring enhanced surface quality. The surface of AISI 321 steel in its standard state reflects light very well, complicating its use for applications requiring low visibility. Therefore, improving the technological foundations for surface roughness formation through femtosecond and nanosecond laser structuring of AISI 321 steel for low-visibility purposes is a relevant scientific task. This research focuses on this issue. The study examines surface modification using laser radiation from nanosecond and femtosecond laser pulses to create both periodic and random structures. Helium-neon laser radiation was used to study the scattering on 3D structures. The types of both periodic and random structures in the scattering spectra were identified, including those that minimize laser radiation reflection.

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# Photosensitizer Properties of $Ti_3C_2$ MXene Under Continuous and Pulsed Regimens of the Near-Infrared Laser

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MXenes, a recently emerged class of 2D transition metal carbides/nitrides, have captured significant scientific interest due to their unique physicochemical properties. These properties offer promising avenues for various applications, including energy storage, water purification, sensors, catalysis and, recently, biomedicine. In particular, MXenes possess uniquely high light-to-heat energy conversion, and therefore they are promising as photosensitizers for non-invasive targeted photothermal therapy (PTT) to cancer treatment. However, there remain unresolved issues related to improving their functional performance, surface functionalities, biocompatibility and biodegradability. Our study aimed to determine and select the optimal laser parameters for PTT with $Ti_3C_2$ MXene on fibroblasts.

During the experiment, we investigated the modes of two types of infrared (IF) lasers: pulse and continuous, using $Ti_3C_2$ MXene at concentrations of 50 ug/ml, 25 ug/ml, 12.5 ug/ml, and 6.25 ug/ml. Human fibroblasts were used as target cells. As a light source, we used a continuous laser with a wavelength of 940 nm (Lica-Surgeon, Photonics Plus LTD, Cherkasy, Ukraine) with an optical light source of 600 μm. Laser processing was carried out at a distance of 30 cm for 10 min at a power of 2 W and four different temporary installations (constant, pulsed with 500 ms ON/100 ms OFF, pulsed with 50 ms ON/50 ms OFF, pulsed with 100 ms ON/100 ms OFF) as well as at a power of 1 W with one temporary installation (constant).

The results of the investigations demonstrated that irradiation at a power of 2 W pulsed (2W 500/100 pulse) and continuously (2W Constant) kills fibroblasts. During the experiment, we proved that the best and safest modes for a pulsed laser: power 2 W with various time settings (pulsed with 50 ms ON/50 ms OFF, pulsed with 100 ms ON/100 ms OFF) and for a constant laser: power 1 W.

Our research highlights the potential of combining photothermal therapy with MXene in cancer therapy.

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# Nanostructuring and Hardening of Subsurface Layers in Structural Steels by Laser Heat Treatment Followed by High-Frequency Mechanical Impact Treatment: Effects of Carbon Content and Alloying Scheme

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**Abstract ID #ULI-1364**

The laser heat (LH) treatment followed by high-frequency mechanical impact (HFMI) treatment effects on the structure and hardness of the gradient-hardened near-surface layers of the carbon and tool steels are studied in this work. The gradient structure is formed in the near-surface layers in the AISI 1045, AISI O2, and AISI D2 steels after the combination of the laser surface transformation hardening followed by the multi-pin ultrasonic impact peening. The multi-pin HFMI treatment provided the nanostructured surfaces hardened by the scan-based LH treatment. The nanostructured steels on the surface with significantly reduced roughness and increased hardness, which can be effective in terms of desired increase in wear and anti-corrosion resistance.

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TRACK 14

# “THEORY &MODELING”

# Predicting Novel 2D $AsBiX_3$ (X = S, Se, and Te) Auxetic Monolayers with Favorable Optical and Photocatalytic Water-Splitting Properties

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**Abstract ID #TM-0918**

The design of two-dimensional multifunctional materials is highly desirable for nanoscale device applications.

In this study, we report the structural, electronic, mechanical, and photocatalytic properties of chalcogenide-based monolayers $AsBiX_3$ (X = S, Se, and Te) using first-principles calculations. The stability of these monolayers is confirmed through energetic and mechanical analyses, as well as ab initio molecular dynamics simulations. The analysis of mechanical properties reveals significant mechanical anisotropy and a bidirectional in-plane negative Poisson ratio in the monolayers. Additionally, the computed electronic band structures, obtained with and without spin–orbit coupling, indicate that these monolayers are indirect-gap semiconductors. At the Heyd–Scuseria–Ernzerhof level, the values of the band gap are determined to be 1.91 eV for $AsBiS_3$, 1.66 eV for $AsBiSe_3$, and 1.32 eV for $AsBiTe_3$. These monolayers have a very high absorbance on the order of ∼5 × 105 cm–1 in the visible and ultraviolet regions with considerable anisotropy. We also found that monolayers hold a high mobility anisotropy. The predicted solar-to-hydrogen efficiency of all monolayers surpasses the critical value (>10%) for the economical production of hydrogen from photocatalytic water splitting. Notably, $AsBiS_3$ and $AsBiSe_3$ monolayers have appropriate band-edge positions that perfectly match the conditions for photocatalytic water splitting at pH = 0, and the band gap and band-edge positions can be adjusted through strain engineering. With these outstanding properties, $AsBiX_3$ (X = S, Se, and Te) monolayers present themselves as promising candidates for applications in optoelectronics, mechanics, and photocatalytic water splitting.

# A Probabilistic Model of Dopant-Induced Spontaneous Phase Separation in Artificial Lipid Membranes: The Case of Two Binding Modes

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Biological membranes are surrounded by water medium containing diversity of compounds, both of endogenous and of exogenous origin, including drug substances. As it was shown in [1] for antibiotic gramicidin S, some compounds may cause spontaneous dopant-induced lipid phase separation into domains with various properties, e.g. the phase transition temperature. An apparent reason for the separation is two modes of gramicidin S binding to lipid membrane, namely, surface-localized and bulk-localized [2]. However, the fact of two binding modes per se seems insufficient to explain lipid phase separation since it could lead to homogeneous distribution of differently bonded dopant molecules.

In the present work, a model of dopant-induced lipid phase separation is suggested which is grounded on a single additional assumption concerning preferential drug binding mode similar to the mode in a local lipid vicinity. Hence, binding probability was higher when dopants with the same binding mode were already present in a local lipid vicinity ("next to similar" probability), and this probability was lower when dopants with another binding mode were present there ("next to other" probability).

The results of computer simulation shown that the abovementioned assumption is sufficient to dopant-induced phase separation, i.e. to appearance emergence of two types of lipid domains with different properties. In particular, such domains become visible when "next to similar" and "next to other" binding probabilities are about 0,95:0,05. In this case, the domains have a complicated, rugged form, weave each other and contain incorporated domains of another type, with general view close to that of a percolation cluster. Rather similar patterns were obtained under Monte Carlo simulation of lipid phase separation in multicomponent membranes [3]. Distribution of the domains area for 0,95:0,05 ratio of the probabilities is power-law on a significant diapason of small-scale area ranges, i.e. it is scale invariant. Simultaneously, if the probability difference is higher, about 0,99:0,01, the domains grow up to the scale comparable to the whole simulated pattern and have smooth, clearly visible boundaries. Commonly, just one domain of each type is present, i.e. the membrane become to be divided into two regions.

Thus, it was shown that a simple mechanism of preference "next to similar" local binding mode is quite enough to arising lipid domains, including those comparable to the size of the system. It should be noted that the finding could occur not only in biological membranes but in any systems, which are similar by its probabilistic properties, – physical, biophysical and probably social.

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# Control of Ferroelectric Domain Structure Formation upon Phase Transition

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The unique physical properties of ferroelectric materials are widely used in modern instrument making: thermal sensors, capacitors, nonvolatile memory and photovoltaics. Formation of ferroelectric domain structure is a nonlinear stochastic process and significantly depends on quenching and relaxation conditions. Numerous kinetic observations of the quenched triglycine sulfate ferroelectric crystal showed that the domain growth and evolution to the thermodynamically stable state takes hours [1,2]. During this time the system is nonequilibrium and sensitive to any even very weak external effects which can contribute the self-assembling formation of domain configuration in demand. But all known experiments were processed till now by Ising approach for the scalar order parameter which is not suitable for polydomain structures with non-zero domain walls.

In this work, we developed a self-consistent theory for describing the domain ordering in uniaxial ferroelectrics after quenching from the paraelectric phase into the ferroelectric one [3]. It allows us to predict all stages of ordering process and control the final state of the domain structure depending on quenching conditions and external fields imposed on the sample during its relaxation to the state of thermodynamic equilibrium. It was found that critical values of control parameters such as quenching temperature and external electric field separating the regions of single-domain and polydomain ordering significantly depend on the quenched disorder and were calculated for different forms of the initial correlation function4. Based on the developed model not only usual kinetic observations of domain ordering but also the enigmatic phenomena such as the strong reduction of charge at the nominally charged "head-to-head" and "tail-to-tail" domain walls were theoretically described [4]. These results allow us to provide methodological guidelines for predicting the process of domain structure formation which opens up the opportunities for creation ferroelectric materials with functional properties in demand.

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# Ab initio Calculations of $ABO_3$ Perovskite Surfaces, Interfaces and Defects Therein

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**Abstract ID #TM-0958**

We performed ab initio calculations for $SrTiO_3$, $BaTiO_3$, $PbTiO_3$, $CaTiO_3$, $SrZrO_3$, $BaZrO_3$, $PbZrO_3$ and $CaZrO_3$ perovskite neutral (001) as well as polar (001) and (111) surfaces [1-3]. For $ABO_3$ perovskite (001) surfaces, with a few exceptions, all atoms of the upper surface layer relax inward, all atoms of the second surface layer relax outward, and all third layer atoms, again, inward. The $ABO_3$ perovskite (001) surface energies always are smaller than the (011) and especially (111) surface energies. The B-O chemical bond population in the $ABO_3$ perovskite bulk always are smaller than near the (001) and especially (011) surfaces. We review our first-principles calculations for STO/BTO, STO/PTO and SZO/PZO (001) interfaces [4]. We analyze the systematic trends in $ABO_3$ perovskite bulk and (001) surface *F*-center ab initio calculations [5]. The calculated formation energy difference between the $ABO_3$ perovskite bulk and (001) surface *F*-centers triggers the *F*-center segregation from the bulk towards the (001) surface.

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# Formation of Heterogeneous Structures in Softened Ice Surface Under Friction

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The study of ice friction is key in physics and other scientific disciplines, as it has a significant impact on a number of natural and artificial processes. Of particular importance for the study of this topic are the processes associated with winter Olympic sports, such as biathlon, figure skating, bobsleigh, etc., where the main sports equipment is in contact with ice [1, 2]. Simulation of these processes helps to better understand the characteristics of ice and its interaction with various objects [1-5]. In recent years, the deformation fields in the ice surface during friction have been actively studied. The key parameters are the shear components of strain and stress, as well as the ice surface temperature [3]. In this work, we further develop a synergetic model that takes into account the spatial heterogeneity of the strain, stress, and temperature of the ice surface layer.

It is shown that in the considered case two types of domains are formed – with positive and negative strain values. The time evolution of the domain structure is studied, and it is shown that over time, the near-surface ice layer becomes homogeneous, and the same value of shear strain is realized over the entire contact area, which determines the relative velocity of the rubbing surfaces. The dependencies of fractal dimensions, domain perimeter, as well as the average domains area and their number on the process time are analyzed. It is shown that it is possible to select the parameters under which the system evolves rapidly to a stationary state, or vice versa, when slow relaxation is observed. The nature of the evolution depends significantly on the initial conditions of the parameters on the contact plane. In the case under consideration, the initial distribution of values is Gaussian, with strain and stress taking both positive and negative values, and temperature taking only positive values. In this paper, we consider a situation where the system becomes homogeneous over time, but it is possible to select parameters under which a deterministic chaos regime is realized, in which the domain structure is constantly changing over time, and a stationary mode of motion is not achieved.

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# Non-Equivalence of Interatomic Interaction in Model Calculations of the Phonon Dispersion

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The consecutive inclusion of additional physical parameters (color, phase, charge sign, spin, etc.) into the symmetrical description led to creation of the theory of color symmetry and the concept of superspatial symmetry [1,2]. Being based on the latter approach, a technique for calculating the phonon dependences of complex crystals has been developed. Among the types of generalized symmetry, the concept of superspatial symmetry is quite convenient and visual when building (3+d) dimensional models describing the structure of complex crystals and systems united by a single metric and the scale of the function of the protocrystal carrier.

Formation of the (3+d) dimensional metric of the protocrystal is based on its higher symmetry and is related with an additional d-dimensional space, which allows the description of real objects (crystals and systems) as natural (sa×sa×sa) superlattices [3]. The use of a complete set of modulation vectors makes it possible to determine the amplitudes of the mass modulation functions and, based on them, to generate a generalized dynamic matrix in the form of a superposition of the protocrystal dynamic matrices, defined at different points of the Brillouin zone, connected by the modulation vectors, as well as in the form of the mass disturbance matrix described by the amplitudes of the mass modulation functions.

The compositional features of the implementation of complex crystals and systems by the mechanism of filling with atoms of different types and vacancies, translationally equivalent positions given by the basis of the protocrystal are covered by the concept of superspatial symmetry [4]. The dynamic matrices of the protocrystal $D\alpha\beta(k + q_i)$ are determined from the relation [4].

It is shown that depending on the choice of the equidistant approximation [3,4] (the force constants are determined only by the distance between the positions of different orbits and do not depend on the type of interacting atoms) and the non-equidistant approximation for the force constants $\alpha_n$ the force constants also depend on the type of interacting atoms) the calculated model phonon spectra of $BaTiO_3$ crystals satisfactorily describe the values of the experimental data in the center of the Brillouin zone (G(Γ)). At the same time, calculations in the equidistant approximation lead to an nonphysical five-fold degeneracy at the point R (value near 25 THz), which is removed at transition to non-equivalent approximation.

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# MXene Property Prediction via Graph Contrastive Learning

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**Abstract ID #TM-1039**

MXenes are an important class of 2-D materials because of their expected novel properties and myriad applications. Some applications include more efficient energy conversion in batteries and solar cells, environmental and water treatment, supercapacitors, electromagnetic interference shielding, and catalysts in chemistry [1]. MXene synthesis is too slow to explore the vast MXene property space [2] - there are likely an infinite number of possible MXenes [1] - necessitating the need for fast methods, such as machine learning methods, that can quickly predict properties and provide guidance to experimentalists. However, existing machine learning methods fail to account for atomic structure information that can be encoded by representing MXenes as graphs - constituent atoms as nodes and bonds between atoms as edges - potentially leading to lower property prediction accuracy.

In this work, we introduce a novel method for predicting MXene properties which uses graph neural networks to predict target features from MXene graph structures and chemical formulas. Specifically, our model uses graph contrastive learning [3], a type of graph neural network method, to transform input features from a graph dataset to a lower-dimensional representation space that enables high-accuracy predictions for downstream machine learning models. We obtain the following RMSEs for downstream models predicting properties from an unpublished MXenes dataset: 0.418 J for Work Function, 0.518 eV−1 for Density of States at Fermi Level, 21.65 N/m for Bulk Modulus, 0.067 for Poisson's Ratio, 14.56 N/m for Shear Modulus, 35.66 N/m for Young's Modulus, and an accuracy of 0.82% for Magnetic (T/F). We also show that, when applied to the molecular QM9 dataset [4], our method obtains lower mean absolute error for predictions of four molecular properties compared with a baseline method of similar complexity [5]. We apply our method to predict important MXene properties which, to the best of our knowledge, have not been successfully predicted by existing deep learning methods that include atomic structure information as model input.

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# Peculiarities of Nanoscale $\alpha$'-phase Precipitation in Fe-Cr-Al Alloys During Thermal Treatment

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Alloys Fe-Cr-Al based on iron are successfully used as cladding materials for fuel elements in nuclear reactors. This is due to their high resistance to oxidation at high temperatures, corrosion and radiation resistance, peculiarities of chemical interaction between fuel and cladding, good mechanical properties. It was shown that increasing the chromium concentration in these alloys can improve their corrosion resistance during operation in high-temperature water reactors, as well as increase resistance to high-temperature steam oxidation; increasing the chromium content leads to potential brittleness of these alloys due to the formation of chromium-enriched $\alpha$'-phase; increasing the aluminum content in the alloys enhances its resistance to high-temperature oxidation, but may increase the temperature of the plastic-brittle transition; adding more than 6 at% aluminum is effective in reducing the stability of the precipitates of the $\alpha$'-phase.

The aim of this work is to investigate the influence of alloying element concentration and annealing temperature on the kinetics of nanoscale $\alpha$'-phase precipitation and its statistical properties during solid solution annealing in the framework of phase-field modeling. We have developed a generalized phase field model for simulating the dynamics of microstructural transformations in Fe-Cr-Al alloys based on iron, taking into account the dynamics of equilibrium point defects using the CALPHAD approach. Within the stability analysis phase diagrams illustrating critical values of annealing temperature and alloying element concentrations at which $\alpha$'-phase precipitates will be stable have been established. The dynamics of precipitate formation from solid solution during thermal treatment has been investigated within the framework of numerical modeling procedure. We analyze the evolution of precipitates number density, average size, volume fraction of precipitates, and chromium concentration in them and the spatial ordering of point defects. It will be shown that during the ripening stage, the average size of precipitates and their number density evolve according to a power law with exponents corresponding to the Lifshitz-Slyozov-Wagner theory. We will show that increasing the concentration of chromium and aluminum initiates phase separation processes, reducing the incubation time for concentration waves development and leading to an increase in the linear size of precipitates and their volume fraction. It will be shown that annealing at elevated temperatures leads to a decrease in the number of precipitates and an increase in their size. Investigating the kinetics of equilibrium point defects, it will be shown that during solid solution annealing, vacancies are mostly uniformly distributed in volume, while interstitial atoms are mostly localized in small $\alpha$'-phase precipitates and inside large precipitates near the phase boundary with high curvature.

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# Universality of Fission-Gas-Bubble Growth in Amorphous Uranium Silicide

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It is known that materials under irradiation are opened systems, where different kind of self-organization phenomena occur: formation of point defect clusters, defect walls, dislocations loops, radiation-induced phase transformations, emergence of cavities and fission-gas-bubbles. These phenomena govern a life-time of these materials and influence safety and performance of commercial and research reactors. Therefore, a study of stability of materials under above non-equilibrium conditions remains an actual problem during last several decades.

In this study a generalized approach to study dynamics of the bubble size at stages of bubble growth and coalescence with the corresponding statistical distributions in amorphous uranium silicide is proposed. It is based on statements of reaction rate theory by taking into account formation of fission-gas clusters, their growth and coalescence effects with a bubble-gas resolution. Scaling properties of both growth and coalescence regimes of nano-sized bubble growth are examined in details analytically and by numerical simulations. It is found that scaling exponents at these regimes are controlled by fission rate and temperature. The nucleation regime is described by the growth exponent close to 1/2, whereas the coalescence regime is characterized by the growth exponent around 1/3. These exponents increase with fission rate and decrease with temperature. The corresponding equilibrium statistical distributions over bubble sizes at these two stages are of universal character. It is shown that nanometer-sized bubbles can change their growth dynamics when their number density exceeds a certain threshold depending on irradiation conditions. Obtained results for crossover of the system dynamics and the swelling correspond well with experimental data. This study provides an insight into details of fission-gas-bubbles growth kinetics in amorphous systems.

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# Effects of Many-Particle Clusters Scattering on Electronic Spectra of Strongly Correlated Alloys in Wannier and Bloch Representations

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**Abstract ID #TM-1078**

A generalizing method for the calculation of electronic structure of disordered systems with strong electronic correlations (SEC), based on the Green's function, is proposed at a temperature of 0 K. It includes the development of the recursive method for the calculating T-matrix of scattering on many-particle clusters for Green's function of the system as well as the extension of this approach to the studying electronic spectra in both direct (Wannier representation) and reciprocal (Bloch representation) space with taking into account the influence of atomic and magnetic correlations and the nanoclusters formation in system. The one-band Hubbard model, the correlated random field approximation, and the one-site approximation of coherent potential for the effective Hamiltonian are used in this method. Calculation of the spectral density in reciprocal space can be carried out by the same way as in direct space, using the corresponding effective Green's function obtained in the case of several sublattices in the crystal. The small parameter of the Green's function cluster expansion in both direct and reciprocal space demonstrates its smallness for different parameters of bcc alloys. This guarantees the convergence of the obtained recursive formulas for contributions to the T-matrix of scattering from many-particle clusters and the applicability of pairwise approximation for the T-matrix. The distributions of the electronic states in the reciprocal (as well as in the direct) space demonstrate a sensitivity to the changes in the energetic characteristics and composition of the alloy components as well as to short-range (nanoscale) magnetic and atomic ordering in the system with SEC. No less promising result is the improvement and development on this basis of experimental methods to the diagnostics of systems with SEC, in particular positron spectroscopy, which provide information about the features of the electronic structure associated with defects, chemical composition and different correlations in the system.

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# Effects of Elastic Interactions Between Adsorbate and Substrate in Nano-Structuring of Thin Films During Deposition

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**Abstract ID #TM-1091**

Nanostructured thin films are garnering increasing attention in both scientific and engineering realms due to their distinct properties, which render them viable for utilization in modern electronic devices. Experimental investigations, analytical treatments, and numerical simulations collectively demonstrate that employing various growth techniques for thin films can lead to patterning on the growing surface. These patterns may manifest as either transient or stationary, contingent upon the control parameters of the system. These parameters typically encompass factors such as the flux of adatoms towards the growing surface, the type of adsorbed particles (i.e., atoms/ions), which dictate the activation energies of adsorption and desorption, and the temperature, among others.

Furthermore, in real-world experiments, multi-layer growth is commonplace, where the minimization principle of surface energy gives rise to a vertical current of adatoms from the top towards the bottom layers. Naively, one might expect the concentration of adsorbate on the bottom layer to consistently exceed that on the top layer. This discrepancy engenders a bias in the standard vertical diffusion of adsorbate between layers. The interplay between these two mechanisms significantly influences the morphology of the growing surface.

In this study, we investigate the role of elastic interaction between the substrate and adsorbed particles in the structuring processes of thin films. We present a reaction-diffusion model for nanostructure formation in the initial deposited layer of a multilayer adsorptive system. Our model accounts for adsorption, desorption, transference reactions between neighboring layers, and nonlinear diffusion. Analyzing a homogeneous system, we demonstrate that increased elastic interaction energy promotes reentrant first-order transitions. We construct a phase diagram illustrating the parameter space for these transitions. Further, by examining the stability of stationary homogeneous states to inhomogeneous perturbations, we show that increased elastic energy induces pattern formation on the growing surface during deposition. We discuss the corresponding stability diagram and analyze the influence of elastic energy on the kinetics of nanostructured thin film growth and the statistical properties of surface structures.

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# Molecular Dynamics of High-Density Polyethylene Composites: Effects of Welding Temperature

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**Abstract ID #TM-1101**

The polyethylene pipes have always played an extremely significant role in gas and water distribution networks because of their numerous advantages [1]. For tightly joining two polyethylene pipe components, thermal butt-fusion welding processes are always the preferred method [2, 3, 4]. The nature of this welding method is to generate temperature-induced physical changes in the welding region of polyethylene, leading it to transition into glassy, rubbery, and viscous states, respectively at various temperatures, respectively [5]. The quality of welding joints is one of the most crucial factors considered, which is typically determined by the heating temperature, heating pressure, and heating time.

The purpose of this study was to investigate the effect of temperature on the quality of welding joints of high-density polyethylene at the molecular level. In this study, the welding system (HDPE polymer model) of MD simulation consists of two parallel molecular chains, each composed of 30 monomers, with a parallel distance of 5Å. The MD (Molecular Dynamics) [6] simulations of energy distribution, geometry optimization, molecular dynamics, and mechanical properties were performed with varying temperature, fixed pressure, and fixed time based on COMPASSIII Forcite in Material Studio 2023. The temperature range investigated spanned from 200°C to 350°C in increments of 30°C, with a fixed pressure of 0.2 MPa and a fixed total simulation time of 150 ps.

This study primarily took the interfacial energy, mean-squared displacement (MSD), radial distribution functions (RDFs) into consideration across different temperatures. By analyzing these results from the MD simulations, the study aims to gain a comprehensive understanding of the effect of temperature on the quality of welding joints of high-density polyethylene from the molecular perspective. Furthermore, research results of this study can also provide certain guidance for high-speed welding of polymers.

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# Plastic Deformation Modeling and Mechanical Properties of Fe-Cr-Al Alloys

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In our study, we focused on investigating the influence of the concentration of alloying elements and the annealing temperature on the mechanical properties of iron-based Fe-Cr-Al alloys. For this aim we carried out the numerical modeling of the plastic deformation processes in the form of simple shear and tension. A generalized model of the phase field with CALPHAD approach was used for samples preparation. The simulations of the applied mechanical loading were performed by using the combination of the phase field method with the nonlinear elasticity theory, that allowed to study the elastic fields evolution and dynamics of defects during the deformation. The modeling was implemented at high values of strain rate from $5\times10^8$ $s^{-1}$ to $10^9$ $s^{-1}$. The deformation curves for previously simulated Fe-Cr-Al alloy samples with different content of chromium and aluminium were obtained and analyzed. It was studied the influence of composition and annealing temperature on the yield strength and ultimate strength. Obtained redistributions of the elastic strain illustrated the formation and evolution of the slip lines. It was analyzed the relative location of slip lines and chromium-enriched precipitates. To determine the strain-rate sensitivity of Fe-Cr-Al alloys, the strain rate influence on the mechanical properties was studied. Obtained results allow to predict changes in the mechanical properties of Fe-Cr-Al alloys depending on the concentration of alloying elements and annealing temperature at different types of mechanical loading and strain rates.

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# Electronic Structure and Luminescence Mechanisms of Phosphate-Based Glass-Ceramic Composites

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**Abstract ID #TM-1194**

The interest in the study of oxide-glass-ceramic composites, in which oxide micro/nanocrystals are incorporated into the oxide-glass matrix, is due to the wide range of potential applications, particularly in electronics, optical thermometry, and biomedical [1]. The physical properties of glass-ceramic materials are largely determined by the electronic properties of the "interfacial region," which has an atomic structure distinct from that of both the crystalline and glass components. The electronic and optical characteristics of interphase regions of composite materials are difficult to predict using only general ideas about atoms, ions or molecules interactions. However, the mutual diffusion of component atoms can be effectively modeled in calculations using the molecular dynamics (MD) methods. Further application of the electronic structure calculation methods to the obtained atomic structures allows to calculate the most important micro- and macro-characteristics of the interphase layers and thus to explain the experimentally observed properties of glass-ceramic composites.

Results of complex computational and experimental studies of the atomic and electronic structures of interphases of oxide glass-ceramic composite materials are presented in this report. Two different types of glass-ceramic composited are considered: a) $KBi(MoO_4)_2$ crystal @ $K_2O$-$P_2O_5$-$MoO_3$-$Bi_2O_3$ glass b) $K_2Bi(PO_4)(WO_4)$ crystal @ $K_2O$-$P_2O_5$-$WO_3$-$V_2O_5$ glass. The atomic structures of interface layers of composites were calculated by MD methods implemented in Amorphous Cell and Forcite programs of Materials Studio software package [2]. The electronic structure calculations were performed in the DFT approximation using the band-periodic plane wave pseudopotential method CASTEP. The excited electronic states and optical spectra of possible centers of luminescence of glass-ceramic composite materials are calculated using the Time-Dependent Density Functional Theory (TD-DFT) within molecular cluster approach.

Obtained computational results are compared with experimental data on structural analysis, optical and luminescence spectroscopy of pure and RE-doped samples of glass-ceramic composite materials synthesized with various content of constituent components and chemical compositions. A relationship between atomic and electronic structures of interface (interphases) layers and optical characteristics of studied composites is analyzed. The possibility of tuning of the optical properties of studied oxide glass-ceramic composite materials is examined. The mechanisms of luminescence in oxide glass-ceramics of different types are discussed.

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# Review of Different Functionals for DFT Calculation of Most Common 2D and Bulk Materials Used in Electronics

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The goal of this work is to present the results of DFT calculations for a large set of materials used in electronics. The key parameter is an energy bandgap. We have calculated this quantity for most common semiconductors (Si, GaAs), wide bandgap semiconductors (GaN, 4H-SiC, h-ZnO, $Ga_2O_3$, AlN, h-BN), semiconductors used for photovoltaics ($Cu_xO_y$, CdSe, CdS, CdTe, ZnTe, GaSb) and other (BaS) as well as 2D materials (graphene, black phosphorus, silicene, germanane). All calculations were done using QuantumATK software [1]. We have focused on the LCAO (Linear Combination of Atomic Orbitals) approach [2] since it has gained popularity since it can deal with nanostructures better than the PW approach and scales much more efficiently than PW with an increasing number of atoms in the structure. We have verified results for different functionals focusing on GGA [3] and hybrid functionals [4] reporting also its computational efficiency. For GGA we have applied PBE functional with and without bandgap correction, whereas for hybrid functionals we have tested HSE06 (Heyd, Scuseria, and Ernzerhof 2006), B3LYP (Becke, 3-parameter, Lee, Yang, and Parr), PBE0 (Perdew, Burke, and Ernzerhof), HSE06DDH functionals [1]. The reason why we focus mostly on the hybrid functionals is that all these functionals are not extensively tested against different materials as the GGA approach.

When considering eg. 4H-SiC, GaN, and ZnO there is no one proper selection of hybrid functionals for accurate prediction of a bandgap for these materials. The popular HSE06 hybrid functional returns energy band gap Eg: 3.18 eV (4H-SiC), 3.39 eV (GaN), 2.67eV (ZnO) when compared with literature data, 3.23 eV (4H-SiC), 3.4 eV (GaN), 3.17-3.44eV (ZnO), fails with prediction of ZnO energy bandgap. For this material the B3LYP hybrid functional returns Eg = 3.24 eV, however, it overestimates the bandgap for 4H-SiC and GaN.

Such discussion would be provided for all materials mentioned above.

We believe that reported results may be a useful guide for the selection of a proper approach when working on DFT simulations.

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# Computer Modeling of Percolating Arrays of Bent Nanotubes

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Filling the insulating host matrix with nanotubes (e.g. carbon) improves noticeably the mechanical properties of the resulting composite. Another remarkable effect is the influence of conductive nanotubes on the electrical properties of the host material. Nanotubes have large length-to-diameter ratio, which plays an important role in the formation of long-range conductive path inside the composite (percolation). The percolation threshold is dependent on many factors, and a number of approaches were developed in order to simulate the process using numerical calculations.

In our previous work we described three-dimensional model of dielectric composite filled with straight nanotubes and calculated the percolation threshold. A system under study is a 3D box filled with 'nanotubes', i. e. conducting cylindrical open-ended tubes of random lengths and thicknesses. For each individual tube it is assumed that length to diameter ratio is chosen randomly from the defined range of minimum and maximum length. The goal of simulations is to determine if there exists a conductive path between the opposite edges of the box.

In the simplest model, the connection between a randomly generated pair of tubes exists when their space coordinates overlap. In real systems, however, tunneling current can flow across two nanotubes that are close enough but not touching. In the present simulations, the tunneling range value is introduced. If the shortest distance between two tubes does not exceed the tunneling range, it is assumed that these two tubes make a tunneling contact. Mathematically, the system is represented as a graph and the percolation search is the search of the connected component of the graph, which contains elements that touch opposite edges of the box ('electrodes'). 'Electrodes' are simulated as pseudo-tubes (having zero dimensions). For the purpose of results saving and data management we have developed a dedicated MS SQL Server database using ADO.NET technology as a database access tool. The results of computer simulations were compared to percolation thresholds experimentally measured for carbon nanotubes dispersed in polyimide composites. For the aspect ratio L/D = 120, experimental threshold is reported at 0.23% volume fraction of the nanotubes. Estimated from our simulations, the respective volume fraction is 0.31%. Considering the relative simplicity of the used model, this is a good agreement between experiment and calculations.

To summarize, computer simulations of conductivity in the framework of the statistical three-dimensional model of 'bent nanotubes' – insulator have been performed. Percolation threshold has been investigated as a function of model parameters. By adjusting the complexity of bending and with taking into account different types of possible connections between individual nanotubes, the satisfactory agreement between simulated and experimental results has been obtained.

# Comparative Analysis of Thyroid Disease Prediction Models Using Machine Learning and Data Mining Techniques and Ensemble Classifiers

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**Abstract ID #TM-1260**

The paper presents a comprehensive investigation into the development of a machine learning model tailored for the prediction of thyroid diseases, underscoring the significance of accurate and timely diagnosis. Leveraging a publicly available dataset from the University of California, Irvine, the study utilizes 29 clinical attributes to construct a robust ML model capable of early symptom detection and thyroid disorder prognosis. It delves into feature analysis, data visualization techniques, and employs cross-validation and synthetic minority oversampling to counter overfitting. Through ensemble learning methods, the model's reliability is reinforced, showcasing high levels of accuracy, sensitivity, and specificity, thus demonstrating its potential for integration into real-time computer-aided diagnostic systems. The research underscores the transformative impact of ML in healthcare, particularly in advancing the management of thyroid-related health conditions.

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# Mechanical Properties Prediction for Polymeric Nanocomposites with Organoclay Nanoadditives

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Recently, many types of nanofillers such as nanoclay, carbon nanotubes (CNTs) and graphene have attracted much interest in research for nanocomposites materials. These materials can be applied in various fields such as aerospace, transportation, automotive, packaging, etc [1-2].

In this paper we present the prediction of the mechanical properties for nano-clays based polymeric nancomposites. The polymeric matrix investigated is PBS, FZ91 and FD92. The Young modulus of the nanocomposite is predicted using the modelling and simulation based Comsol Multiphysics software.

A simplified micromechanical model of a particulate composite is presented. A representative volume element (RVE) based on a predetermined particle spacing is assumed to represent the microstructure of the composite. The homogenized elastic properties of the composite material are computed based on the individual properties of the particles and the matrix. The composite is assumed to be made of a periodic microstructure identified as a primitive parallelepipedal structure. A unit parallelepiped RVE have a parallelepiped particle (the flake of nano-additive) embedded in the center of the matrix. Although the thickness of a single flake is about 1 nm, we considered the thickness as a variable in our model, due to possible agglomeration of several flakes into a cluster.

We have to mention that the Young's modulus of the polymer matrix and of the flakes strongly influence the nanocomposite simulated Young's modulus. In order to define the dimensions of the unit cell, a length for the polymer matrix and a thickness of the flakes (we suppose the flakes are staked to form a scaled nm thickness together) were fixed. Such that we varied them keeping the length of the flakes at 100 nm x 100 nm. After fixing the geometry of the unit cell we performed new simulations in order to obtain the Young's modulus (elasticity matrix) results when the concentration of flakes in the polymer matrix is varied.

Finally, a comparison between the modelled mechanical properties and the experimental measurements values was performed.

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# Spectroscopic Theories and First-principles Calculations for Using Rare-Earth Ions Doped in Nanofabricated Materials to Build Quantum Computers: Showcases of $RE^{3+}$ Doped $Y_2SiO_5$

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Without using any trapping lasers, rare-earth (RE) ions can be doped into some nanofabricated materials in form of nanocrystals in a solid state matrix, thus rendering a natural trap for potential application as a quantum computing device [1,2]. In particular, passive nuclear spin states of RE ions can be utilized as (i) optical quantum memory (with huge density as yielded from nanocrystals), (ii) qubits by encoding in ground hyperfine states and operated as (iii) two-qubit gate when transferring them to active magnetized electronic states. A feasible implementation of qubits is realised by using those doped RE ions whose open-shell (for inner highly shielded 4f shell electrons) energy levels and statevectors are well described by the crystal field (CF) interaction and hyperfine coupling in which the Hamiltonian is composed of various free-ion interactions, the CF potential, electronic and nuclear Zeeman effects as well as the hyperfine interaction. For those qubit encoded in the two ground hyperfine states of RE ions, they can have fairly long lifetimes of days and coherence times (from 1.3s for $Er^{3+}$ to 6 hours for $Eu^{3+}$) due to the unique spectroscopic properties of RE ions. Because of the recent progress in optical single-ion detection [3,4] for addressing individual qubits with a specific frequency channel, RE ions could be packed in a solid state 3D matrix at nanometer spacing, hence rendering very high qubit densities for quantum memories. Meanwhile, this configure also leads to strong dipole-dipole interactions (or high connectivity) between qubits which are not nearest neighbors [1,2].

In this study, Kramers ions like $^{167}Er$ and $^{171}Yb$ doped in yttrium orthosilicate $Y_2SiO_5$ (YSO) nanocrystals [5] will be investigated as a promising system for quantum computing because of their weak spin bath and possibility for being directly milled in single nanocrystals as nano-resonators. By using the famous Wien2k package to carry out the first-principles calculations, we can obtain the CF parameters and hyperfine constants as well as various electronic properties like energy gap and band structure for several Kramers RE ions doped in YSO. Based on those calculated results, we shall present our predicted findings on various properties of the ground and excited CF and hyperfine states for those RE ions with an aim to optimize RE ions doping in YSO nanocrystals for quantum memories and qubits, contributing to scalable quantum computing architectures.

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# Computational Studies of Nanomaterials for Electrochemical Energy Conversion and Storage

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Renewable energy as an alternative to conventional fossil fuels is a long-standing goal which will have a revolutionary impact in all aspects of energy utilization. Understanding electrochemical processes involved in interconversion of chemical and electrical energy is key for new generations of technologies such as fuel cells, batteries and CO2 reduction. These processes, e.g. electrochemical water splitting driven by renewable energy sources , often rely on expensive platinum group metals (PGM). Decades of research in developing alternatives to PGM highlight challenges in finding stable and scalable electrocatalysts.

First-principles electronic structure calculations provide valuable insights on the origins of the activity and stability of electrocatalysts. In particular, we investigated several promising nanostructured electrocatalysts with superior activity and stability. A hierarchical electrocatalytic structure of Ni3S2 nanorods which are then decorated with ultrathin MoS2 and Co9S8 nanosheets unique integrated CoMoNiS-NF nanoassembly, whose superior activity is very promising for water electrolysis over a wide pH range. Calculations suggest that Co9S8/MoS2 has enhanced electrochemical activity than Co9S8 by itself because of (a) charge transfer from Co to MoS2, (b) the resulting higher oxidation state of Co, and (c) different binding energies of reaction intermediates.

One of the design concepts for new electrocatalysts is dynamically stable materials, which can couple the stability of a PGM-free electrode material with the activity of dynamic species present in the electrolyte to achieve the required functionality in key water electrode cycle reactions, such as the oxygen reduction reaction. Demonstration of this concept by studying the activity–stability trends for the oxygen evolution reaction on conductive M1OxHy, Fe– M1OxHy and Fe–M1M2OxHy hydr(oxy)oxide nanoclusters (M1 = Ni, Co, Fe; M2 = Mn, Co, Cu) involves balancing the rates of Fe dissolution and redeposition over a MOxHy host to establish dynamically stable Fe active sites [2]. Our model of the electrochemical interface between a perovskite oxide and the electrolyte involves an electronic conductive ABO3 core that allows surface evolution and formation of the hydr(oxy)oxide shell, where the active and dynamically stable Fe(aq) species promote oxygen evolution [3].

## ACKNOWLEDGMENTS

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TRACK 15

# “INTERDISCIPLINARY & MISCELLANEOUS TOPICS”

# Utilising the Interactions Between Bacteria and Magnetite Nanoparticles for the Potential Application in Irish Agricultural Lands

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The interactions between magnetic iron oxide nanoparticles (IONPs) and bacteria occur mostly via electrostatic and hydrophobic attractions [1]. As a result of these interactions, the physical and biochemical properties of bacteria alter depending on the type of bacteria. Due to the superparamagnetic property of magnetic nanoparticles, the bacteria-nanoparticles system can be manipulated by an external magnetic field. This feature can be implemented in biological matrices such as food, soil and water [2]. The association of beneficial bacteria and magnetite nanoparticles [3] can be applied to Irish agricultural soils followed by optimization to increase soil fertility.

This study first aims to investigate the interactions between $Fe_3O_4$@Citrate NPs with model bacteria. Subsequent findings will be applied/ tested upon soil bacteria (including PSB) isolated from Irish peatlands which will be screened for biofertilizer qualities. The study focuses on evaluating the effect of co-application of IONPs with PSB in Irish agricultural soil to be used as a potential nano-biofertilizer.The chemical synthesis of IONPs was confirmed by XRD, DLS, VSM and TEM. IONPs' capacity to capture *Bacillus cereus*, E.coli, *Salmonella typhi* and *Staphylococcus aureus* was evaluated. The particle concentration-dependant and time-dependant studies were employed to optimise the effect of concentration and time required to form bacteria-IONP interactions. Growth kinetics were observed for Bacillus cereus-IONP interactions. The effect of IONPs on cell membrane permeability and nuclei acid leakage will be examined. Bacterial species isolated from Irish peatlands were primarily tested for their affinity to IONPs.Synthesized IONPs were spherical with an average hydrodynamic size of 52 nm. XRD analysis confirmed six indicator peaks for citrate stabilized IONPs. *Bacillus cereus* showed the highest capture efficiency (95.8%) by IONPs while *Staphylococcus aureus* exhibited the lowest (86.3%) capture efficiency. Therefore, *Bacillus cereus* was chosen for the following experiments. As IONP concentration increased (0.125-4.0 mg/mL), the magnetic extraction of bacterial cells increased while the viability of cells decreased. Significant inhibition ($p = 0.0136$) of growth was observed at 2.0 and 4.0 mg/mL of IONP (43 and 45% respectively). However, a growth-promoting effect on bacteria was observed at a minute concentration of IONP (0.125 mg/mL) in this study. As the time of magnetic exposure increased, the cell number in the supernatant decreased to < 1 within 175 seconds. Bacterial species isolated from peatlands demonstrated different affinities towards different concentrations of IONPs. Follow-up studies will anticipate utilizing similar types of interactions with peat microbiota for land application. The effect of encapsulation of PSB with IONPs on the level of soil fertility will be studied.

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# A DFT Study Of $TPPS_4$ Monomers, Dimers and Their Absorption Spectra

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Recently there has been growing interest in $TPPS_4$ for applications in photodynamic therapy. The 5,10,15,20-tetrakis(4-sulfonatophenyl) porphyrin (TPPS4) molecules have been extensively studied because they efficiently self-associate from monomers to large J- or H- aggregates in aqueous media depending on the compound concentration and pH value. The dominant form of $TPPS_4$ depends on the pH of the solvent: $H_2TPPS_4^{4-}$ dominates in alkaline (pH $\approx$ 12) and neutral solutions (pH $\approx$ 7), $H_4TPPS_4^{2-}$ dominates in a pH range of $\approx$ 4 – 3, $H_6TPPS_4^{0}$ is prevalent at a pH of $\approx$ 1, and $H_8TPPS_4^{2+}$ appears to dominate at even lower pH. It is still not clear what type of aggregates are formed in specific conditions.

In this work, we show that monomeric forms dominate at pH = 12.1, pH = 7.1, pH = 4.1, pH = 3.0, and pH = −1.0, in contrast, J-type dimers become a dominant form at pH = 1.0. These results coincide with the literature reporting that $TPPS_4$ (in a form where a half of the peripheral $SO_3^-$ groups is replaced by $SO_3H$) tends to form J-aggregates in acidified aqueous solutions. This is because of the electrostatic repulsion being weakened between $TPPS_4$ molecules in the acidic solution (pH < 2) [1]. These quantum chemistry (it was used DFT CAM-B3LYP/6-31G(d,p) and PCM method) studies suggest an aggregate seeds structure at the molecular level. A number of structural transformations of $TPPS_4$ have been determined when changing the acidity from pH = 12.1 to pH = −1.0. It reveal that five different forms of $TPPS_4$ monomers and ten dimers were found as possible candidates for aggregate precursors. Theoretically calculated absorption spectra coincide with experimentally measured spectra [2]. According to our calculations, the aggregation is related to zwitterion formation, and the growth proceeds starting from Z2 ($SO_3H$ groups are adjacent) monomers.

## ACKNOWLEDGMENTS

Computations were performed on resources at the supercomputer "VU HPC" of Vilnius University in the Faculty of Physics location.

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# X-ray Irradiation Time Behavior of Exciton Luminescence for Yttria Sintered from Nanosized Powder

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**Abstract ID #IMT-1104**

$Y_2O_3$ (yttria) as a crystalline nanomaterial attracts an attention in biomedicine, optics and optoelectronics, especially fiber laser and amplifier development, display panels and fluorescence lamps etc. The known luminescent patterns of Y2O3 when stimulated by different forms of ionizing radiation have been extensively studied, and one of the predominant features is the emission linked to self-trapped exciton decay. Previous research from our team has demonstrated that long-term irradiation of nano-sized $Y_2O_3$ ceramics by 60 keV X-rays led to changes in the exciton wavelength band [1]. So we developed the quantitative physical model of an exciton luminescence of polycrystalline $Y_2O_3$ basing on photoelectron trapping by intergrain pores and caverns of the polycrystalline sample [1].

But within the framework of our model, some questions still remained unsolved, why exactly such a functional dependence of the decrease in the exciton luminescence intensity over time, whether there are factors that influence it. Here we performed a mathematical treatment of the experimental data set to establish the functional dependence and also developed our theoretical model. The experimental time dependence of exciton luminescence intensity at photon energies of 3.1, 3.56 and 4.13 eV for the ceramics sample sintered from $Y_2O_3$ nano-sized powder was accurately examined by means of analysis and processing of the data through the fitting procedure. Optimal alignment between the observed luminescence intensity dynamics and the fitted outcomes was attained by employing a time-dependent model featuring two exponential components. The outcomes of the fitting procedure can be explained by the existence of two categories of traps, each characterized by its capacities and the rates at which trapped electrons relax. According to the SEM-data for our samples (both for plane surface and fresh cleavage), most of the caverns have a characteristic size of the same order as the grains, while a significantly smaller number of caverns with a characteristically larger size. We suggest that the largest contribution to the decrease in luminescence level is provided by a set of cavities that have relatively small dimensions comparable to the grain sizes. A smaller contribution is made by relatively large cavities, which are also characterized by a lower relaxation rate of trapped electrons. A simple physical model is proposed to explain the fact that the relaxation rate of trapped electrons is higher for small cavities.

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# The Stamped Coal Nanoblend Coking: Law Regulation and Industrial Technology Development Features

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**Abstract ID #IMT-1107**

Modern industrial coking technologies provide for the production of high-quality blast furnace coke from blends that must contain at least 50% of well-coking coals [1]. At the same time, the largest share of coking coal reserves in the world is gas coal [2], which has limited use in coking blends. The technology of stamping is one of the main special methods of preparing coal blends to increase the coke production economic indicators. The legal regulation peculiarities to ensuring environmental industrial enterprises' safety through the development of stamped blends coking technologies in Ukraine are considered [3]. The effective industrial technologies development for the coking stamped blends coking , taking into account the environmental requirements for industrial production, using the coke production waste - float concentrates and sludges from coal processing plants, is very important.

The obtained coke was subjected to destructive forces for the realization of cracks by dropping it 4 times from a height of 1 m onto a metal plate, after which the coke was calibrated on sieves with round holes with a diameter of 70, 60, 50, 40, 25 and 10 mm. Based on the results of screening, the yield of individual size classes was calculated. The amount of coal with size <0.5 mm in the coal blends was 48.3-58.0% due to the addition of float concentrate and sludge, which contained up to 90% coal with size <0.5 mm.

A comprehensive study of the coking raw material base components properties was carried out. Based on this, several options for coal blends composition were developed and experimentally tested. The coal nanoblend during stamping, in addition to meeting the general requirements for obtaining high-quality coke, must have sufficient stamping capacity. Compositions of coal blends have been developed, which make it possible to obtain a stamped cake with required strength and high-quality coke on mastered designs coke ovens batteries. Proposed requirements for stamped coal nanoblend for coking chambers of increased height. It is justified that in order to increase the height of the furnace for coking the stamped blend, a proportional increase in the strength of the stamped cake is necessary. This ensures the stability of the cake when it is loaded into the coking chamber and prevents complications in the furnace's operation.

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# Fast Photoactuation of pDAP / Silicon Cantilevers

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We demonstrate the fabrication of poly(diaminepropane)-coated Si cantilevers through a plasma polymerization technique and their use as photothermal, humidity-driven actuators. The developed pDAP films exhibit high elasticity with Young's modulus ranging between 6.5 and 8 GPa, and remarkable mechanical durability across temperatures from 20 to 80 °C. Notably, the pDAP layer of merely 50 nm thickness can be freely suspended over a millimeter-sized opening, showcasing an impressive length-to-thickness ratio of approximately 40,000. The pDAP layers respond to multiple stimuli including atmospheric moisture, temperature, and laser light which we employ for tunable deflection of cantilevers.

Our study shows robust dynamic characteristics of pDAP/silicon beams when stimulated via photothermal heating. The determined relaxation times owing to water sorption remain below 10 ms, and relaxation times owing to thermal expansion are of the order of 40 µs enabling the actuation at frequencies from 10 Hz to 1 kHz. The demonstrated light-to-motion conversion opens exciting possibilities for future applications based on biocompatible and standard technologies.

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# Metal Nanoparticles as Maize Growth Promoters, Evaluation of their Antimicrobial Activity and Potential Phytotoxicity

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In the context of sustainable development, effective solutions to increase agricultural productivity are being required. Nanotechnology provides new alternatives, including nanomaterials for effective delivery of nutrients and enhancement of plant resistance to abiotic and biotic stresses or control of pathogens and pests [1]. The understanding of the interaction of nanoparticles with plants is essential to identify their potential to growth stimulation, while also determining the risk of toxicity [2]. Therefore the aim of this study was to evaluate the effect of biologically synthesized zinc oxide (ZnONPs) and silver nanoparticles (AgNPs) on *Zea mays* seeds germination, seedlings growth and condition.

The ZnONPs and AgNPs were synthesized by using fungal extract from *Fusarium solani* IOR 825 and their size, crystalline structure, functional groups on their surface, size distribution and surface potential were evaluated by using Transmission Electron Microscopy (TEM), X-ray Powder Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FTIR) and Nanoparticle Tracking Analysis (NTA), respectively. The maize seeds were nanoprimed with bio-NPs solutions at concentrations of 32, 128 and 512 µg $mL^{-1}$ and cultivated for 14 days at ± 22°C. The germination percentage (%G), mean germination time (MGT), germination rate index (GRI), length, fresh and dry biomass were analyzed. The seedling condition was estimated by determination of vigour indexes (I and II) and the chlorophyll content in bio-NP-treated seedlings. Moreover, antimicrobial activity of bio-NPs was evaluated by determination of minimal inhibitory and minimal biocidal concentration (MIC and MBC) values against plant pathogens.

Results showed no effect on seed germination and dose-dependent effects of bio-NPs on maize seedlings growth. The treatment with both bio-NPs the concentration of 32 and 128 µg $mL^{-1}$ (ZnONPs) and 512 µg $mL^{-1}$ (AgNPs) resulted in increase of fresh and dry biomass of seedling shoot and root. as well as higher values of vigour index I and II by 8-12% and 15-29%, respectively. The reduced chlorophyll content by 12-13% was observed in seedlings treated with ZnONPs (at concentrations of 128 and 512 µg $mL^{-1}$) and AgNPs (at concentration of 512 µg $mL^{-1}$). The highest antibacterial activity was observed for AgNPs against Pseudomonas syringae IOR 2188 (MIC=8 µg $mL^{-1}$ and MBC = 512 µg $mL^{-1}$) and for ZnONPs against Xanthomonas camperstris IOR 512 (MIC=256 µg $mL^{-1}$ and MBC=2048 µg $mL^{-1}$).

The use of bio-NPs for seed impregnation results in improved maize biomass production and phytopathogen control. The application of low concentrations of bio-NPs revealed no adverse effect on seeds germination, seedling condition or chlorophyll content, indicates their potential for use in agriculture as nano-agrochemicals to provide nutrients and protection against microbial pathogens.

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# Assessment of Airborne Nanoparticles Exposure and Risk Management Strategies During the Life Cycle of Multi-Materials with a Nanocomponent: Flamingo Project Case Studies

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Engineered nanoparticles production and incorporation in new products have been increasing worldwide, due to the nano-scale enhanced material properties. During nanoparticles life cycle, workers, the general population and even the environment can be potentially exposed to engineered nanoparticles, which might lead to serious health effects in a medium to long term.

Many efforts have been made to develop suitable frameworks, tools and models, to support nanoparticles exposure assessment and risk management in occupational settings, considering the complex relationships between variables in the nanotechnology field and the lack of occupational exposure data and occupational exposure limits (OELs) [1]. Workplace exposure assessments have shown that release and exposure to airborne nanoparticles depends on the characteristics of the nanomaterial and the working process itself [2].

Considering the uncertainties and complexity of assessing the Health effects and the risks of airborne nanoparticles to human health, the potential sources of airborne nanoparticles release and pathways that workers may be exposed during the nanoproduct value chain in the FLAMINGo project have been analysed. The FLAMINGo project (GA nº101007011) aims to develop a highly efficient production of advanced multi-materials with a nanocomponent and introduce them in the conventional metallurgical and forming industrial technologies for production of electric vehicle components. The nanoproduct value chain from formulation to the recycling phases of aluminium metal matrix nanocomposites is under study.

This work aimed to assess the potential release and emissions of ultrafine particles during the formulation, manufacturing, processing and recycling phases of the nanoproduct, under development in FLAMINGo. To distinguish between the emissions sources related to the activities of the nanoproduct life cycle and the background (BG), measurements were mainly performed before, during and after the activities, following the recommendations of ISO [3, 4] and using real-time monitoring equipment. The obtained data was analysed and the critical points, with the highest nanoparticles emissions, were identified and workers exposure significance was determined according with the criteria established by NanoGEM project [5] and EN [6].

Our results indicate the need of implementing proper filters in the ventilation systems, such as high efficiency particulate air (HEPA) filters with class H13 or H14, to remove the airborne nanoparticles before venting to a safe place outside the building, as they provide a collection efficiency close to 100% in the nanoparticles size range. An overview of the general good practices and risk management strategies proposed in the cases studied in FLAMINGo are given to raise safety awareness among value chain stakeholders of nanoproducts focused on the need to assess the nanoparticles risks on a case-by-case basis and to adopt risk prevention-based approaches.

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# Mapping of Geometric Characteristics of Overlay Welded Walls of Aluminum Alloy AA5087

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In the contemporary context of seeking more cost-effective and adaptable approaches to metal component production, the Wire and Arc Additive Manufacturing technique (WAAM) is gaining prominence. Over the past decade, the advanced WAAM method, as a subset of additive manufacturing (AM), has garnered considerable attention and application [1,2]. This technique employs metal welding wire as the feedstock (on the welding process side), an electric arc as the heat source (on the AM technology side), and computer-based control (on the automation side). Traditional AM-produced metal products often suffer from porosity issues, limiting their full utilization. Consequently, this technology presents a promising solution to address these challenges. This study aimed to map the geometric characteristics of overlay welded walls of aluminum alloy, focusing on the influence of gas flow rate. The substrate material utilized was AA5083 aluminum alloy, while AA5087 aluminum alloy served as the filler material. The substrate plates were sized at 100 × 200 × 20 mm, and the wires had a diameter of 1.2 mm. An experimental investigation was conducted at various levels of gas flow rates (8, 10, 12, and 14 l/min) to analyze their effects on the width of the weld bead, weld height, fusion area, and penetration depth into the substrate. Macroscopic analysis was performed emphasizing potential impacts of different gas flow rate levels. Additionally, the waviness of individual overlay welds was examined through macroscopic analysis. As the gas flow increased, the height of the layer also increased due to cooling. The highest layer height was measured in layers fabricated with a gas flow rate of 14 l/min, reaching 2.247 mm. The lowest waviness of the layers was achieved at a gas flow rate of 12 l/min. The maximum effective width of the layer was found at a gas flow rate of 8 l/min, namely 6.26 mm. The results of this study provide a detailed insight into the impact of gas flow rate on the geometric characteristics of overlay welded walls of aluminum alloy AA5087 and offer valuable insights for optimizing the welding process. Studying the behaviour of aluminum alloy in the overlay welding process under various parameters of gas flow rate during welding can lead to broader applications of this technology in the industry, through which it would be possible to eliminate geometric defects and porosity. Simultaneously, it can enable improvements in cost-effective production, for example, in the automotive, shipbuilding, and aerospace industries, which are its primary objectives [3,4].

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# The Influence of Interlayer Waiting Time on the Temperature Distribution in Aluminium Alloy made with Wire and Arc Additive Manufacturing

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Wire and Arc Additive Manufacturing (WAAM) is becoming a new progressive technique for the production of various metallic components by means of deposition „layer by layer". WAAM is characterized by high deposition rates, relatively simple equipment, and high material utilization, thus decreasing the material waste in comparison to other production technologies. Furthermore, WAAM is suitable for the production of medium to large structural components, such as cruciform, stiffened panels, and wing ribs [1]. When applying WAAM for the production of the aluminium alloys components, excessive heat accumulation could be encountered. The heat accumulation leads to the dendrite and grain coarsening resulting in the decrease in mechanical properties of printed parts. Furthermore, when the heat accumulation is too high, the humping of the component could occur, which makes impossible to print defect free component with required properties. This defect will be copied to the next deposited layers and will lead to the destruction of the part. There are several approaches how to reduce the heat accumulation in the aluminium alloy parts being WAAMed [2]. Research is currently focused on several ways of improvement in mechanical properties like application of special cooling equipment [1], interlayer friction stir processing [3] or application of interlayer hammering [4]. On the other hand, mentioned approaches could prolong the production times of WAAM process. Adjusting the waiting time between deposition of each layer could be another efficient approach of possible elimination of overheating the printed part. The influence of various interlayer waiting times on the geometry of walls and temperature distribution was investigated. Cold Metal Transfer (CMT) based WAAM process was used for the production of 5087 aluminium alloy walls. The waiting times between deposition of individual layers ranging from 0 to 120 seconds were. The interlayer waiting times 0, 30, 60, 90, and 120 seconds were used for production of walls. Strategy of movement of the CMT torch in alternating directions was used for the deposition of walls. The thermal cycles were measured during the deposition of each aluminium alloy wall. Furthermore, the surface temperatures distribution of individual layers was monitored. Based on the reached results, it can be stated that the increase in the interlayer waiting time resulted in the decrease in the maximum temperature measured during WAAM. The longer the interlayer waiting time, the higher the cooling rate. Furthermore, the different interlayer waiting times resulted in the change in geometrical characteristics of deposited walls, namely the effective width of the printed walls. The longer the interlayer waiting time, the narrower the effective thickness of the produced wall.

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# Metal Nanoparticle-enhanced Polymer Gel Dosimeters for FLASH Beam Dose Measurements

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FLASH (ultra-high dose rate) radiation therapy holds promise for improved treatment outcomes. Potential benefits include reduced damage to healthy tissue surrounding tumors, faster treatment times, and minimized dose delivery errors [1, 2]. However, dosimetry for ultra-high dose rate beams remains an under-investigated area, particularly with less frequently used techniques like polymer gel dosimetry. This technique is attractive due to high spatial resolution and ability to provide volumetric dose distribution information [3].

This study investigates the response of various polymer gel dosimeters containing silver (Ag) nanoparticles as sensitivity enhancers to ultra-high dose rate electron irradiation. The ultra-high dose rate electron beam was acquired by modification of Varian TrueBeam medical linear accelerator. The results were compared with irradiation using conventional dose rates. The study shows similar response of polymer gel dosimeters irradiated with conventional and FLASH dose rates. This observation was further supported by Fourier Transform Infrared (FTIR) spectroscopy, which evaluated radiation-induced structural changes in gels. These findings on dose response under ultra-high dose rate irradiation show a potential of Ag enhanced polymer gel dosimeters to be used as a beam characterization and dose measurement tool for FLASH therapy.

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# Integrated Strategies for Enhancing the Maturity of hiPSC-Derived Cardiomyocytes: A Molecular, Metabolic, and Morphological Approach

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In recent years, cardiomyocytes derived from human-induced pluripotent stem cells (hiPSC-CMs) have proven invaluable for modeling inherited cardiac diseases and advancing patient-specific, non-invasive therapies. However, a significant challenge lies in the cultivation of mature 2D cardiac tissues that accurately reflect human heart physiology. This is due to hiPSC-CMs often displaying immature functional and morphological traits, such as a rounded shape and inconsistent beating rates. Given the limited in-depth studies on enhancing maturity, our objective is to integrate various strategies—molecular, metabolic, and morphological—to emulate some of the key physiological characteristics of adult ventricular cardiomyocytes. Our approach includes molecular maturation, achieved by adding specific small molecules (cyclic AMP and 3,3',5-Triiodo-L-thyronine) to the culture medium. Metabolically, we aim to transition the cells from a purely glycolytic metabolism, characteristic of immature cells, towards a more physiological metabolism where fatty acids contribute to 60-70% of cardiac energy production. Additionally, we use micropatterned coverslips to restrict cell growth and promote fiber-like alignment in hiPSC-CMs, thereby enhancing cell-cell contact and promoting maturation. By assessing the organization of sarcomeric proteins (cardiac troponin I, α-actinin, and myosin heavy chain) through immunofluorescence and multiphoton second harmonic generation imaging—and evaluating contractility parameters via video-edge detection—our preliminary results show promising improvements, particularly in the alignment of sarcomeres in hiPSC-CMs. However, the treatment with fatty acids to enhance β-oxidation has shown mixed results, with no significant improvement in the surface area or organization of the hiPSC-CMs sarcomeres.

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# Towards Real-time Quality Control in Spark-Assisted Chemical Engraving (SACE) Process

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Glass is widely utilized in microfluidics owing to its inherent properties, transparency, and biocompatibility. Among various techniques for fabricating glass microchannels, Spark-Assisted Chemical Engraving (SACE) emerges as a non-traditional effective method. SACE operates through an electrochemical phenomenon, generating high-energy discharges by immersing a tool electrode within an electrolyte and applying a high voltage, facilitated by a hydrogen gas film that isolates the tooltip. Discharges cause local heating to the temperature of around 650oc, causing high-temperature etching. SACE has demonstrated the capability to produce microchannels with surface roughness as low as 0.3 µm at an acceptable machining speed that reaches 200 µm/s. Critical properties such as microchannel texture, dimensions, and geometric consistency significantly influence their functionality in fluid dynamics and heat transfer applications. Despite the notable advantages of SACE, the technique exhibits inherent uncertainties and nonlinear behaviors, and there remains potential for further improvement to obtain more predictable outputs that meet specific shape and texture requirements. Addressing the unpredictable nature and irregular relationship between process parameters and machining quality, this study extracted SACE process signatures (gas film formation time and mean discharge energy) by current signal processing with time series classification to establish a correlation between these parameters so that a more robust predictive model is developed. This research introduces a model that controls the process signatures by adjusting the machining voltage parameters, including amplitude, period, and duty cycle. By utilizing a precision machine that maintains a constant tool travelling rate and gap during microchannel machining and is equipped with real-time hardware, the SACE machine with controlled process parameters can produce microchannels with uniform surface roughness and consistent geometries. In the future, developing a closed-loop control model incorporating more robust techniques and additional control elements could compensate for the SACE's uncertainties, making a faster and more efficient method for glass microchannel fabrication.

# Plasmonic Enhancement of Photosensitizing Properties of Hybrid Three-Component Nanosystem Anionic Polyacrylamide/Gold Nanoparticles/Temoporfin

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**Abstract ID #IMT-1277**

Photodynamic therapy is a type of medical treatment that works by combining a special photosensitizing agent with light and molecular oxygen to evoke cell death. After absorbing light of an appropriate wavelength, photosensitizer undergoes a type I or type II photochemical reaction, generating either free radicals or reactive oxygen species (ROS). Such ROS and radicals damage surrounding cells, leading to either necrosis, apoptosis or autophagy. Such treatment has less side effects compared to traditional methods of chemotherapy and radiotherapy [1], however, the are some limitations, namely poor water solubility and some level of dark cytotoxicity of most photosensitizers, as well as their nonselective accumulation in non-target tissues.

In our work, we studied a three-component hybrid nanosystem that consists of star-like dextran-graft-polyacrylamide anionic polymer-nanocarrier, gold nanoparticles and temoporfin photosensitizer. Encapsulating photosensitizers in nanocarriers helps to improve biocompatibility, selectivity, bioavailability, and phototherapeutic effects, as well as the stability and hydrophilicity of a drug [2]. Another increasingly popular approach that we adopted in this work for enhancing drug's anti-tumor efficiency is addition of metal nanoparticles. Namely, it was discovered that gold nanoparticles can be used to substitute and complement many chemotherapeutic drugs improving therapeutic responses [3]. Also, metal nanoparticles are well known and widely used to enhance various optical processes such as surface-enhanced Raman scattering (SERS), absorption (SEA), fluorescence (SEF), and photocatalysis by using the phenomenon of surface plasmon resonance.

We have performed optical characterization and analysis of the mentioned triple nanosystem, and observed significant enhancement of ROS generation compared to bare temoporfin. We have also determined optimal concentrations of the components which provides maximum photodynamic efficiency of developed hybrid nanosystem.

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# The Use of Nanopowders of Refractory Compounds in Welding

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The process of metal modification is traditionally used in the production of steel castings to obtain a fine-grained structure, increase strength, ductility and impact toughness. However, the use of material modification with dispersed powders has not been widely used in microelectronics, additive manufacturing, and even welding. This is due to a number of factors, and above all, to the difficulties that arise when introducing modifiers into liquid metal during its production or welding.

Recently, a number of publications have appeared which show the feasibility of introducing nanosized particles of refractory compounds into the metal melt to modify the weld metal in the process of crystallization and microstructure formation [1-3]. One of the effective mechanisms of structure modification is related to the increase of crystallization centers of the metal melt due to the use of flux-cored wires of different fillings during welding [4, 5].

The purpose of this work was to investigate the influence of nano-sized up to 100 nm refractory particles of the oxide type on the formation of the microstructure and mechanical properties of the weld metal of HSLA steels. The article investigates the peculiarities of the formation of the metal microstructure of welds of low-alloy steels when nano-sized particles of refractory oxides $Al_2O_3$, $TiO_2$, MgO, $ZrO_2$ are added to the melt. It is shown that the inoculation of oxides with a low level of mismatch of the crystal lattice with the lattice of δ-ferrite and increased wetting of nanoparticles (MgO, $ZrO_2$) contributes to the growth of new dispersed phases that are formed during melt crystallization.

The work established that the use of MgO and $ZrO_2$ nanooxides contributes to the increase in the size of dendrites formed during the crystallization of the welding bath. It is shown that the onset of austenite disintegration in weld metal inoculated with MgO and $ZrO_2$ nanooxides begins at lower transformation temperatures. The increased stability of primary austenite grains can be related to the morphology of dendrites that formed at the beginning of the crystallization process. In weld metal inoculated with $TiO_2$ and $Al_2O_3$ nanooxides, the formation of the bainite structure begins at temperatures below the temperature at which austenite disintegration begins. Under these conditions, there is an increased diffusion of carbon from the austenite grains, which leads to the enrichment of ferrite phase precipitates at the boundaries of the primary austenite grains with carbon. Modification of the metal of the welding bath with $TiO_2$ and $ZrO_2$ nanooxides contributes to the formation of the acicular ferrite structure. An increase in the content of needle ferrite in the microstructure of the weld metal contributes to an increase in the level of strength and ductility of the welds.

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